10/ 075,909

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS	4	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	5	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	6	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	7	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	8	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Righ Truncation
NEWS	9	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	10	SEP 22	DIPPR file reloaded
NEWS	11	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	12	SEP 29	DISSABS now available on STN
NEWS	13	OCT 10	PCTFULL: Two new display fields added
NEWS	14	OCT 21	BIOSIS file reloaded and enhanced
NEWS	15	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced

NEWS EXPRESS	OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
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FILE 'HOME' ENTERED AT 11:14:44 ON 28 OCT 2003

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:15:00 ON 28 OCT 2003
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 OCT 2003 HIGHEST RN 609766-09-8
DICTIONARY FILE UPDATES: 27 OCT 2003 HIGHEST RN 609766-09-8

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

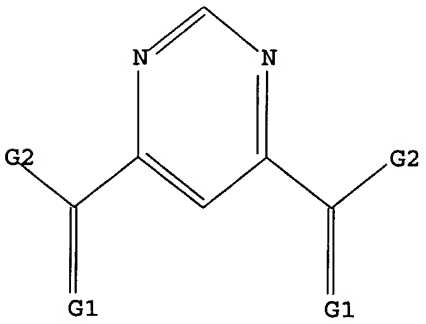
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10075909.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

G2 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
FULL SEARCH INITIATED 11:15:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1506 TO ITERATE

100.0% PROCESSED 1506 ITERATIONS 118 ANSWERS
SEARCH TIME: 00.00.01

L2 118 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.15	148.36

FILE 'CAPLUS' ENTERED AT 11:15:41 ON 28 OCT 2003
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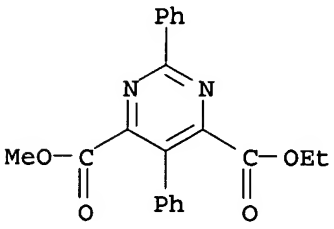
FILE COVERS 1907 - 28 Oct 2003 VOL 139 ISS 18
FILE LAST UPDATED: 27 Oct 2003 (20031027/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l2
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L2 ANSWER 1 OF 118 REGISTRY COPYRIGHT 2003 ACS on STN
RN 605686-66-6 REGISTRY
CN 4,6-Pyrimidinedicarboxylic acid, 2,5-diphenyl-, ethyl methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H18 N2 O4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s l2
L3 27 L2

=> d l3 1- ibib abs hitstr
YOU HAVE REQUESTED DATA FROM 27 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:696859 CAPLUS
DOCUMENT NUMBER: 139:230480
TITLE: Preparation of substituted amines prodrugs useful in

10/ 075,909

treating Alzheimer's disease

INVENTOR(S): Varghese, John; Jagodzinska, Barbara; Maillard, Michel; Beck, James P.; Tenbrink, Ruth E.; Getman, Daniel

PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn

SOURCE: PCT Int. Appl., 483 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072535	A2	20030904	WO 2003-US7287	20030227

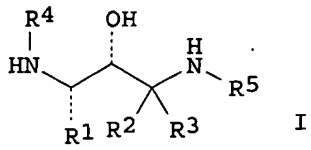
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

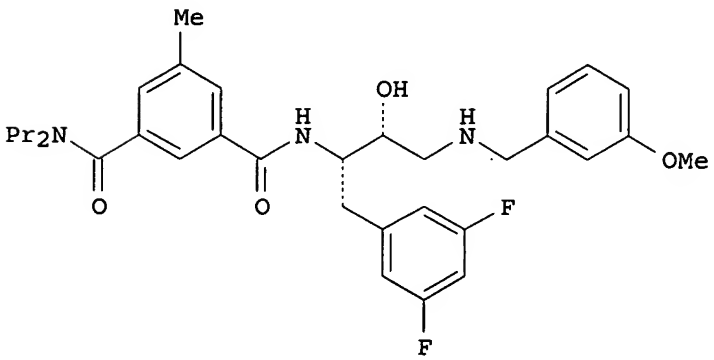
PRIORITY APPLN. INFO.: US 2002-359953P P 20020227

OTHER SOURCE(S): MARPAT 139:230480

GI



I



II

AB Amines [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, (un)substituted alkyl, alkenyl, etc.; R3 = H, (un)substituted alkyl, alkenyl, etc.; R4 = XR; X = CO, SO2, a bond, etc.; R = Ph, naphthyl, indanyl, etc.; R5 = (un)substituted alkyl, (CH2)0-3cycloalkyl, etc.; e.g. N1-[(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-[(3-methoxybenzyl)amino]propyl]-5-methyl-N3,N3-dipropylisophthalamide], useful in treating Alzheimer's disease and other similar diseases, were prepd. Although the methods of prepn. are not claimed, hundreds of example

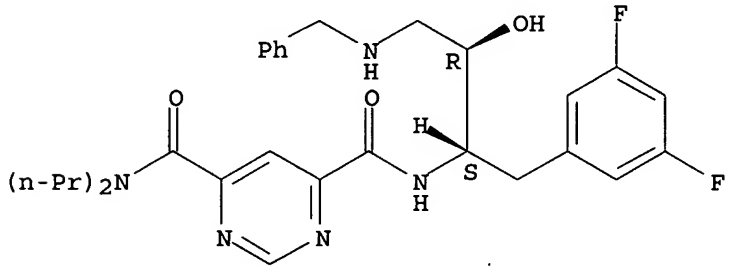
prepns. are included. Thus, reacting (2R,3S)-3-amino-4-(3,5-difluorophenyl)-1-[(3-methoxybenzyl)amino]-2-butanol trifluoroacetate with 5-methyl-N,N-dipropylisophthalamic acid in the presence of Et3N, 1-hydroxybenzotriazole and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride in DMF afforded (1S,2R)-II (N1-[(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-[(3-methoxybenzyl)amino]propyl]-5-methyl-N3,N3-dipropylisophthalamide). The compds. I exhibit an IC50 of < 50 .mu.M against .beta.-secretase.

IT **388063-71-6P**, N-[(1S,2R)-3-(Benzylamino)-1-(3,5-difluorobenzyl)-2-hydroxypropyl]-N',N'-dipropyl-4,6-pyrimidinedicarboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of substituted amine prodrugs useful in treating Alzheimer's disease)

RN 388063-71-6 CAPLUS

CN 4,6-Pyrimidinedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-2-hydroxy-3-[(phenylmethyl)amino]propyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:563735 CAPLUS

DOCUMENT NUMBER: 139:276843

TITLE: 2H-Azirines as dipolarophiles

AUTHOR(S): Pinho e Melo, Teresa M. V. D.; Cardoso, Ana L.; Gomes, Clara S. B.; Rocha Gonsalves, Antonio M. d'A.

CORPORATE SOURCE: Faculdade de Ciencias e Tecnologia, Departamento de Quimica, Universidade de Coimbra, Coimbra, 3004-535, Port.

SOURCE: Tetrahedron Letters (2003), 44(33), 6313-6315
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

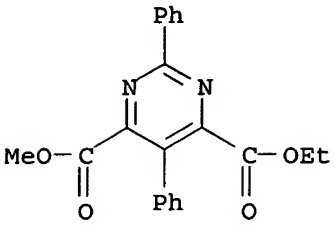
LANGUAGE: English

AB 2H-Azirine-3-carboxylates unsubstituted at C-2 act as dipolarophiles in the reaction with diazomethane giving new 4,5-dihydro-3H-pyrazole derivs. The synthesis of a pyrimidine was also achieved via 1,3-dipolar cycloaddn. of Me 2-bromo-3-phenyl-2H-azirine-2-carboxylate with an azomethine ylide.

IT **605686-66-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pyrimidine deriv. via 1,3-dipolar cycloaddn. of Me bromophenylazirinecarboxylate with azomethine ylide)

RN 605686-66-6 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, 2,5-diphenyl-, ethyl methyl ester (9CI) (CA INDEX NAME)



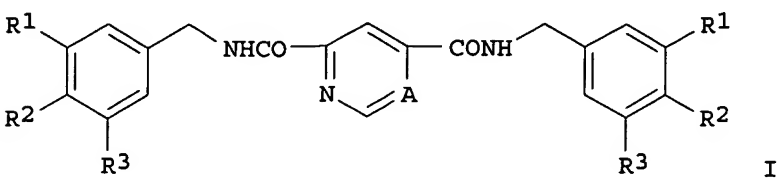
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:467290 CAPLUS
DOCUMENT NUMBER: 139:53028
TITLE: Preparation of 2,4-pyridinedicarboxamides and 4,6-pyrimidinedicarboxamides as inhibitors of collagenase (MMP 13)
INVENTOR(S): Habermann, Joerg; Weithmann, Klaus-Ulrich; Kogler, Herbert; Kirsch, Reinhard; Wehner, Volkmar
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10160357	A1	20030618	DE 2001-10160357	20011208
WO 2003049738	A1	20030619	WO 2002-EP13240	20021125

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2001-10160357 A 20011208
OTHER SOURCE(S): MARPAT 139:53028
GI



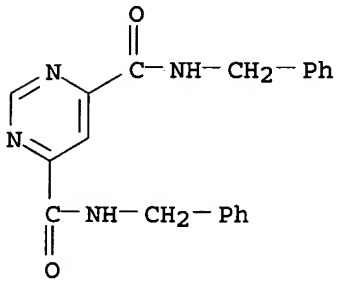
I

AB Title compds. [I; A = CH, N; R1-R3 = H, halo, (halogenated) alkyl, alkoxy, OH, CO2R4, cyano, NR5R6, etc.; R4 = H, alkyl; R5, R6 = H, alkyl, alkylcarbonyl, etc.; or R1R2, R2R3 = 5-6 membered (arom.) (satd.) (hetero)cyclyl], were prepd for the treatment of degenerative joint

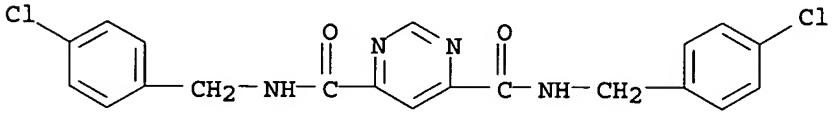
diseases. Thus, 4,6-pyrimidinedicarboxylic acid in SOCl2 was stirred for 2 h at 85.degree. followed by addn. of CH2Cl2 at room temp. and Et3N at 0.degree.. The reaction mixt. was further stirred with 3-chloro-4-fluorobenzylamine for 15 min to give 40% N,N-bis(3-chloro-4-fluorobenzyl)pyrimidine-4,6-dicarboxamide. The latter inhibited collagenase 3 (MMP 13) with IC50 = 23 nM.

IT **135002-40-3P 448949-33-5P 448949-34-6P 448949-35-7P 448949-36-8P 544678-67-3P 544678-69-5P 544678-70-8P 544678-75-3P 544678-76-4P 544678-78-6P 544678-79-7P 544678-80-0P 544678-81-1P 544678-82-2P 544678-83-3P 544678-84-4P 544678-85-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridine- and pyrimidinedicarboxamides as inhibitors of collagenase (MMP 13))

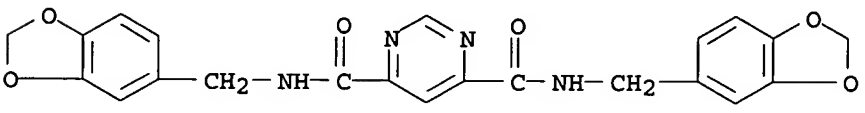
RN 135002-40-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



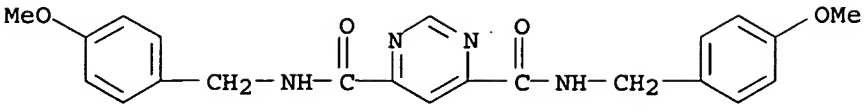
RN 448949-33-5 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



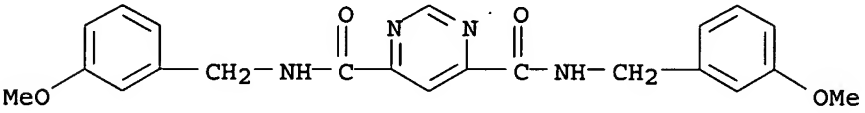
RN 448949-34-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(1,3-benzodioxol-5-ylmethyl)- (9CI) (CA INDEX NAME)



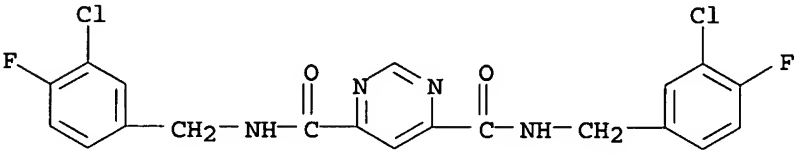
RN 448949-35-7 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



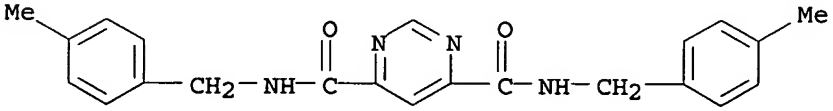
RN 448949-36-8 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



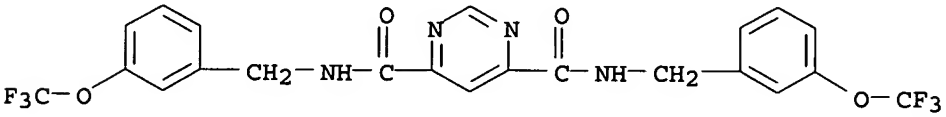
RN 544678-67-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



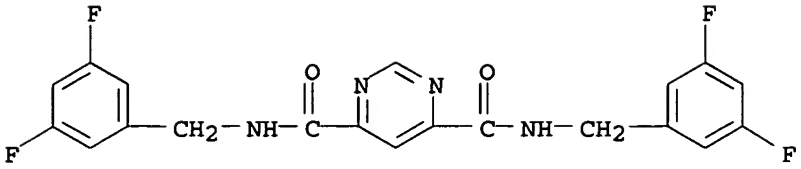
RN 544678-69-5 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



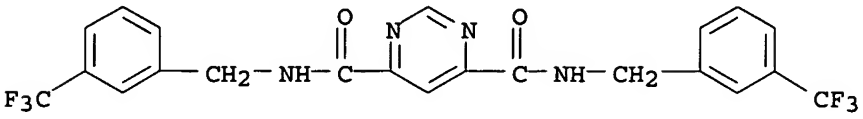
RN 544678-70-8 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[[3-(trifluoromethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



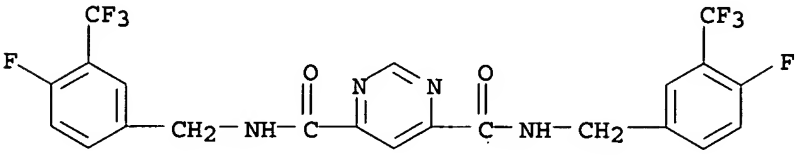
RN 544678-75-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3,5-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



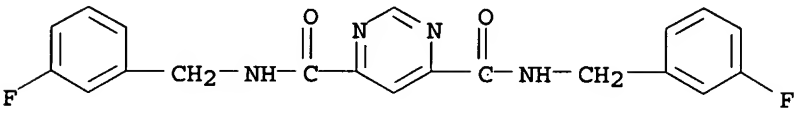
RN 544678-76-4 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



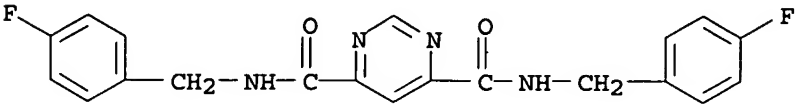
RN 544678-78-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[[4-fluoro-3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



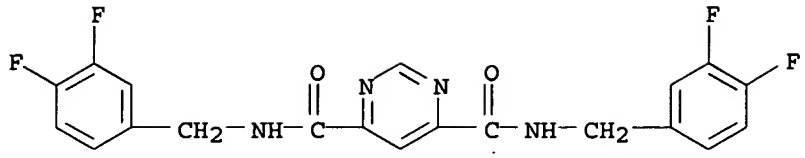
RN 544678-79-7 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 544678-80-0 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 544678-81-1 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 544678-82-2 CAPLUS
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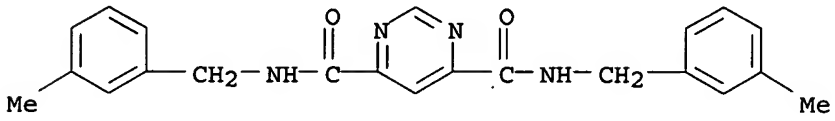
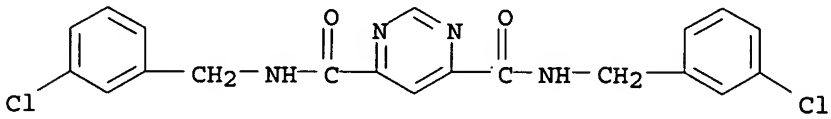
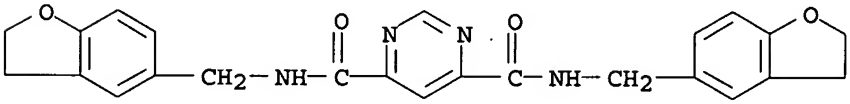


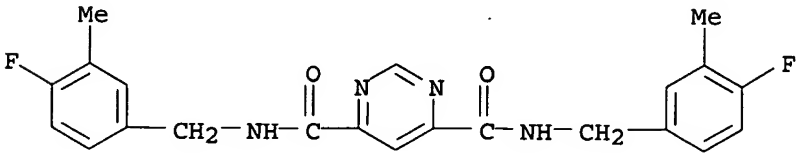
RN 544678-83-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



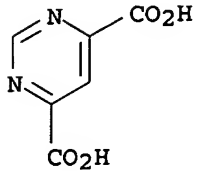
RN 544678-84-4 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(2,3-dihydro-5-benzofuranyl)methyl]- (9CI) (CA INDEX NAME)



RN 544678-85-5 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-fluoro-3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

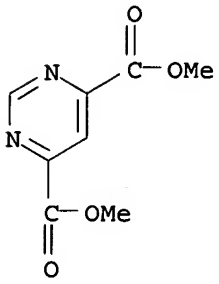


IT **16490-02-1**, 4,6-Pyrimidinedicarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyridine- and pyrimidinedicarboxamides as inhibitors of collagenase (MMP 13))
RN 16490-02-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

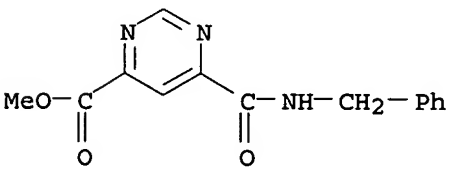


IT **6345-43-3P 544678-86-6P 544678-87-7P**
544678-88-8P 544678-89-9P 544678-90-2P
544678-91-3P 544678-92-4P 544678-93-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridine- and pyrimidinedicarboxamides as inhibitors of collagenase (MMP 13))

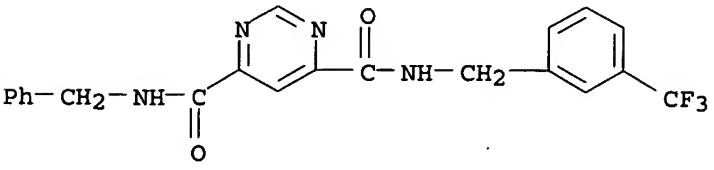
RN 6345-43-3 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



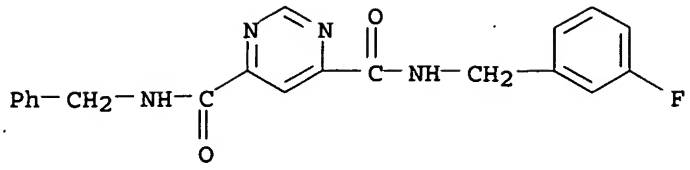
RN 544678-86-6 CAPLUS
CN 4-Pyrimidinecarboxylic acid, 6-[[(phenylmethyl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



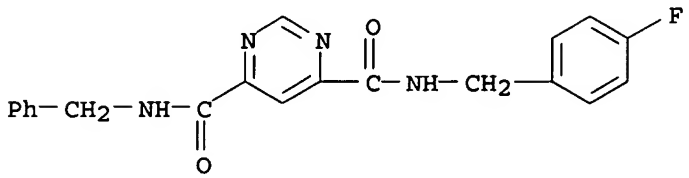
RN 544678-87-7 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-(phenylmethyl)-N'-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



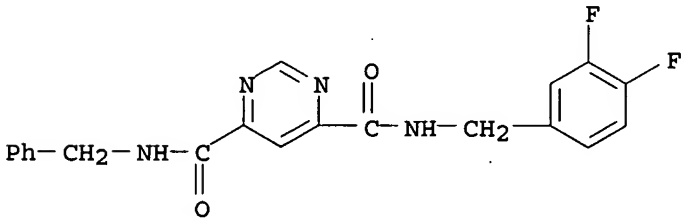
RN 544678-88-8 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-[(3-fluorophenyl)methyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



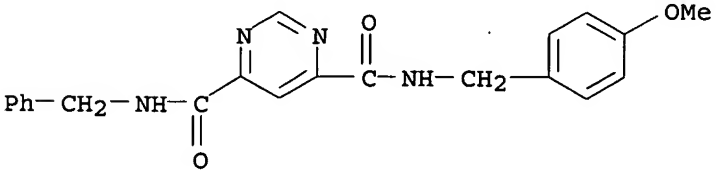
RN 544678-89-9 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-[(4-fluorophenyl)methyl]-N'-(phenylmethyl)-
(9CI) (CA INDEX NAME)



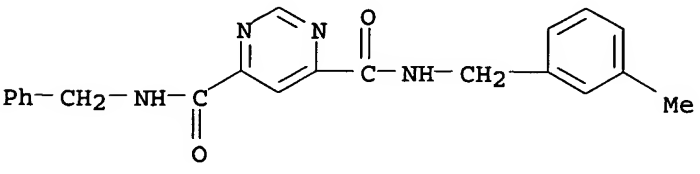
RN 544678-90-2 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-[(3,4-difluorophenyl)methyl]-N'-
(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 544678-91-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-[(4-methoxyphenyl)methyl]-N'-(phenylmethyl)-
(9CI) (CA INDEX NAME)



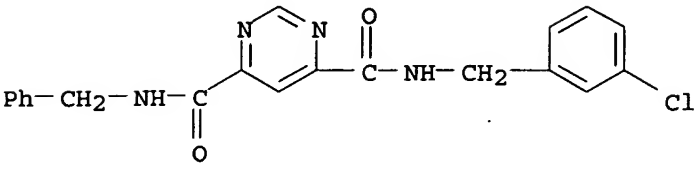
RN 544678-92-4 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-[(3-methylphenyl)methyl]-N'-(phenylmethyl)-
(9CI) (CA INDEX NAME)



RN 544678-93-5 CAPLUS

10/ 075,909

CN 4,6-Pyrimidinedicarboxamide, N-[(3-chlorophenyl)methyl]-N'-(phenylmethyl)-(9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:221564 CAPLUS
DOCUMENT NUMBER: 138:256226
TITLE: Proton-conducting membranes and their use
INVENTOR(S): Calundann, Gordon; Sansone, Michael J.; Uensal, Oemer; Kiefer, Joachim
PATENT ASSIGNEE(S): Celanese Ventures Gmbh, Germany
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022412	A2	20030320	WO 2002-EP9629	20020829
WO 2003022412	A3	20030912		
W: BR, CA, CN, JP, KR, MX, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
DE 10144815	A1	20030327	DE 2001-10144815	20010912

PRIORITY APPLN. INFO.: DE 2001-10144815 A 20010912

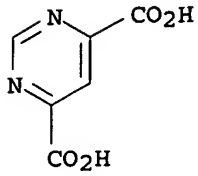
AB The title membranes, with high sp. conductivities, esp. at temps. >100.degree., and esp. useful in fuel cells (no data), are prepd. by dissolving polyazoles in polyphosphoric acid (I) at .ltoreq.400.degree., casting the solns. on supports, and treating the resulting membrane until it is self-supporting. A soln. of 10 g polybenzimidazole (inherent viscosity 0.92 dL/g) in 90 g I (P2O5 content 83.4%) was prepd. under N at 270.degree., thinned with 33.33 g 85% H3PO4, cooled to 240.degree., cast on a glass plate preheated to 100.degree. to a 150 .mu.m film, and left for 3 days under ambient conditions (resulting in hydrolysis of I) to give a mech. stable film with inherent viscosity 1.68 dL/g and sp. cond. 0.115 and 0.128 S/cm at 25 and 160.degree., resp.

IT **471257-03-1 471257-07-5**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(proton-conducting membranes and their use)

RN 471257-03-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, polymer with [1,1'-biphenyl]-3,3',4,4'-tetramine (9CI) (CA INDEX NAME)

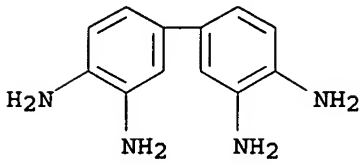
CM 1

CRN 16490-02-1
CMF C6 H4 N2 O4



CM 2

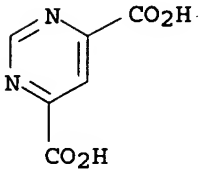
CRN 91-95-2
CMF C12 H14 N4



RN 471257-07-5 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, polymer with 1,2,4,5-benzenetetramine (9CI) (CA INDEX NAME)

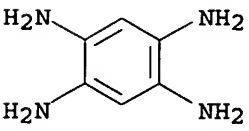
CM 1

CRN 16490-02-1
CMF C6 H4 N2 O4



CM 2

CRN 3204-61-3
CMF C6 H10 N4



L3 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:793682 CAPLUS
DOCUMENT NUMBER: 137:311964
TITLE: Proton-conducting membrane and the use thereof for fuel cells
INVENTOR(S): Calundann, Gordon; Sansone, Michael J.; Uensal, Oemer;

10/ 075,909

	Kiefer, Joachim
PATENT ASSIGNEE(S):	Celanese Ventures G.m.b.H., Germany
SOURCE:	PCT Int. Appl., 51 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM.. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002081547	A1	20021017	WO 2002-EP3901	20020409
W: BR, CA, CN, JP, KR, MX, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 10117687	A1	20021017	DE 2001-10117687	20010409

PRIORITY APPLN. INFO.: DE 2001-10117687 A 20010409

AB Proton-conducting membranes based on polyazoles, useful as polymer electrolyte membranes in fuel cells at >100.degree., are manufd. by dissolving the polyazoles in polyphosphoric acid and forming membranes.

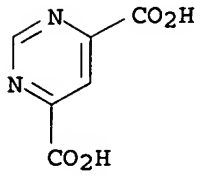
IT **471257-03-1 471257-07-5**
RL: TEM (Technical or engineered material use); USES (Uses)
(polyphosphoric acid-doped; proton-conducting membranes from polymer electrolytes based on polyphosphoric acid-doped polyazoles)

RN 471257-03-1 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, polymer with [1,1'-biphenyl]-3,3',4,4'-tetramine (9CI) (CA INDEX NAME)

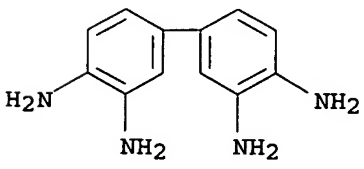
CM 1

CRN 16490-02-1
CMF C6 H4 N2 O4



CM 2

CRN 91-95-2
CMF C12 H14 N4



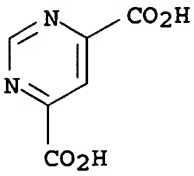
RN 471257-07-5 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, polymer with 1,2,4,5-benzenetetramine (9CI) (CA INDEX NAME)

CM 1

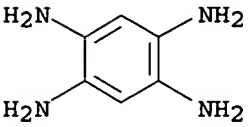
10/ 075,909

CRN 16490-02-1
CMF C6 H4 N2 O4



CM 2

CRN 3204-61-3
CMF C6 H10 N4



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:637659 CAPLUS
DOCUMENT NUMBER: 137:185500
TITLE: Preparation and formulation of pyrimidine-4,6-dicarboxamides as MMP-13 inhibitors
INVENTOR(S): Barvian, Nicole Chantel; Patt, William Chester
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064571	A1	20020822	WO 2002-IB190	20020118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002151555	A1	20021017	US 2002-75909	20020213

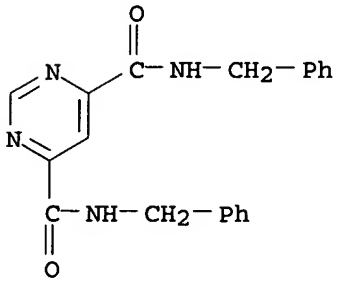
PRIORITY APPLN. INFO.: US 2001-268779P P 20010214
OTHER SOURCE(S): MARPAT 137:185500
AB Z[C(:X)R]2 [each R independently = OR4 or NR4R5; R4,R5 = H, alkyl, (hetero)aryl, etc.; NR4R5 = heterocyclyl; X = O or S; Z = 2-(un)substituted pyrimidine-4,6-diyl] were prepd. as MMP-13 inhibitors (no data). Thus, pyrimidine-4,6-dicarboxylic acid was amidated by

PhCH2NH2 to give pyrimidine-4,6-dicarboxylic acid bis(benzylamide).

IT **135002-40-3P 448949-19-7P 448949-20-0P**
448949-21-1P 448949-22-2P 448949-23-3P
448949-24-4P 448949-25-5P 448949-26-6P
448949-28-8P 448949-30-2P 448949-31-3P
448949-32-4P 448949-33-5P 448949-34-6P
448949-35-7P 448949-36-8P 448949-37-9P
448949-38-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and formulation of pyrimidine-4,6-dicarboxamides as MMP-13 inhibitors)

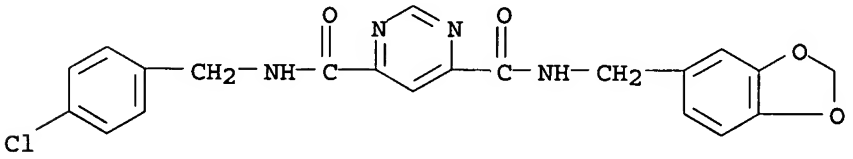
RN 135002-40-3 CAPLUS

CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



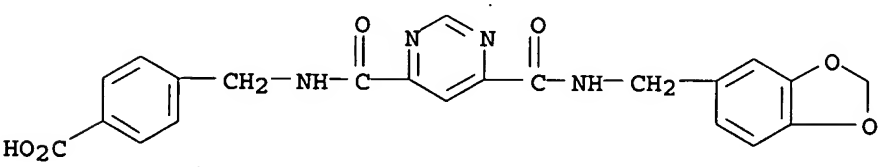
RN 448949-19-7 CAPLUS

CN 4,6-Pyrimidinedicarboxamide, N-(1,3-benzodioxol-5-ylmethyl)-N'-[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



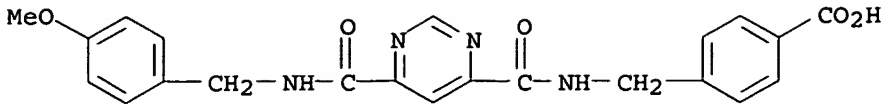
RN 448949-20-0 CAPLUS

CN Benzoic acid, 4-[[[[6-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

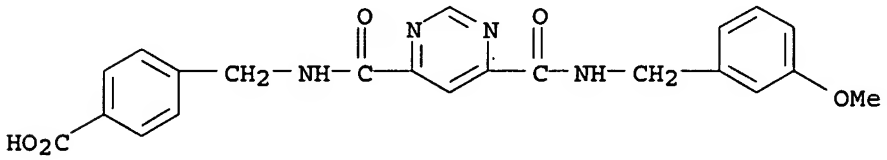


RN 448949-21-1 CAPLUS

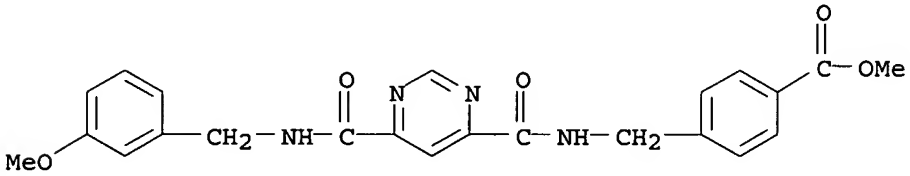
CN Benzoic acid, 4-[[[[6-[[[(4-methoxyphenyl)methyl]amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



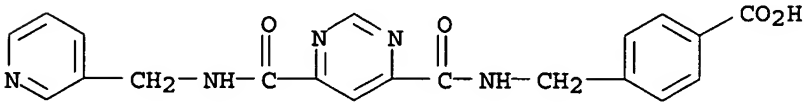
RN 448949-22-2 CAPLUS
CN Benzoic acid, 4-[[[[6-[[[(3-methoxyphenyl)methyl]amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



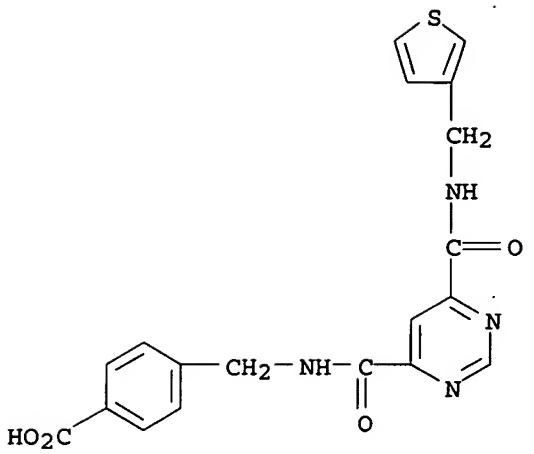
RN 448949-23-3 CAPLUS
CN Benzoic acid, 4-[[[[6-[[[(3-methoxyphenyl)methyl]amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)



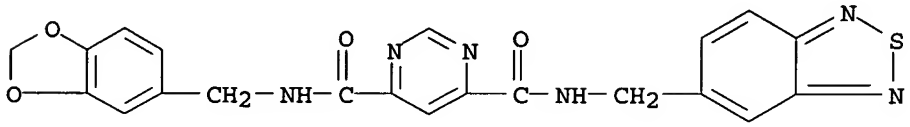
RN 448949-24-4 CAPLUS
CN Benzoic acid, 4-[[[[6-[[(3-pyridinylmethyl)amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



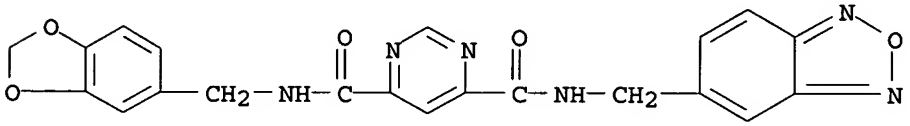
RN 448949-25-5 CAPLUS
CN Benzoic acid, 4-[[[[6-[[(3-thienylmethyl)amino]carbonyl]-4-pyrimidinyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



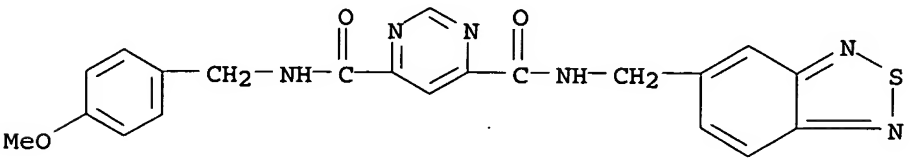
RN 448949-26-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-(1,3-benzodioxol-5-ylmethyl)-N'-(2,1,3-benzothiadiazol-5-ylmethyl)- (9CI) (CA INDEX NAME)



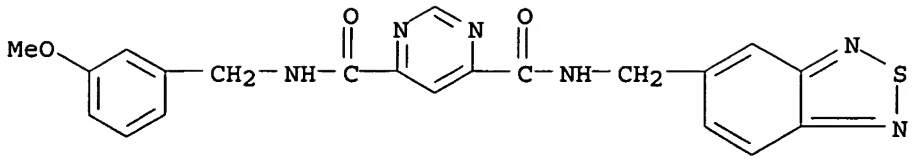
RN 448949-28-8 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-(1,3-benzodioxol-5-ylmethyl)-N'-(2,1,3-benzoxadiazol-5-ylmethyl)- (9CI) (CA INDEX NAME)



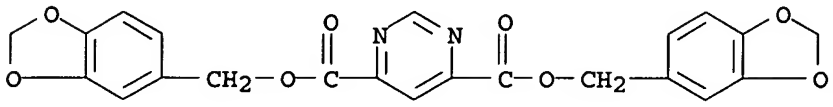
RN 448949-30-2 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-(2,1,3-benzothiadiazol-5-ylmethyl)-N'-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



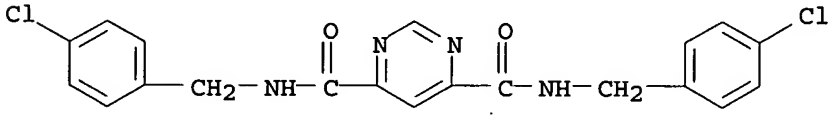
RN 448949-31-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N-(2,1,3-benzothiadiazol-5-ylmethyl)-N'-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



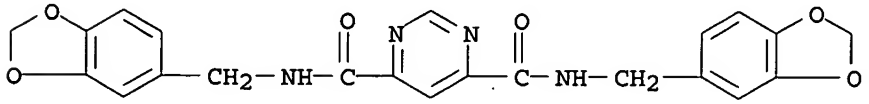
RN 448949-32-4 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, bis(1,3-benzodioxol-5-ylmethyl) ester (9CI) (CA INDEX NAME)



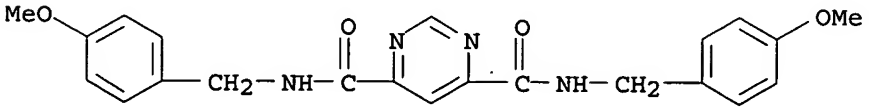
RN 448949-33-5 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



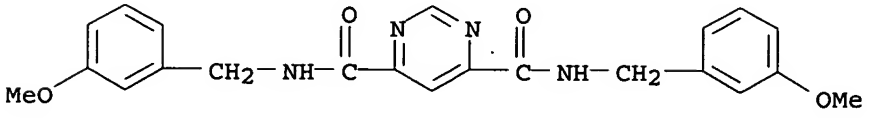
RN 448949-34-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(1,3-benzodioxol-5-ylmethyl)- (9CI) (CA INDEX NAME)



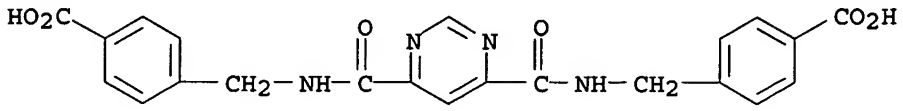
RN 448949-35-7 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



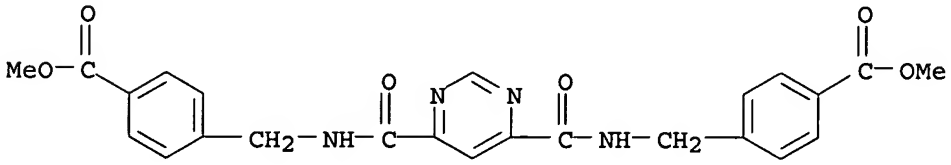
RN 448949-36-8 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



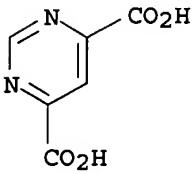
RN 448949-37-9 CAPLUS
CN Benzoic acid, 4,4'-[4,6-pyrimidinediylbis(carbonyliminomethylene)]bis- (9CI) (CA INDEX NAME)



RN 448949-38-0 CAPLUS
CN Benzoic acid, 4,4'-[4,6-pyrimidinediylbis(carbonyliminomethylene)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



IT **16490-02-1**, 4,6-Pyrimidinedicarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and formulation of pyrimidine-4,6-dicarboxamides as MMP-13 inhibitors)
RN 16490-02-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:31402 CAPLUS
DOCUMENT NUMBER: 136:102190
TITLE: Preparation of substituted amines to treat Alzheimer's disease
INVENTOR(S): Maillaird, Michel; Hom, Court; Gailunas, Andrea; Jagodzinska, Barbara; Fang, Lawrence Y.; John, Varghese; Freskos, John N.; Pulley, Shon R.; Beck, James P.; Tenbrink, Ruth E.
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SOURCE: PCT Int. Appl., 651 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

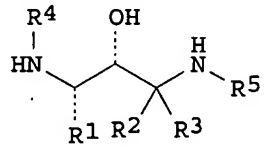
WO 2002002512	A2	20020110	WO 2001-US21012	20010629
WO 2002002512	A3	20030821		
W:	AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
US 2002128255	A1	20020912	US 2001-896139	20010629
BR 2001012000	A	20030603	BR 2001-12000	20010629
EP 1353898	A2	20031022	EP 2001-952378	20010629
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
NO 2002006199	A	20030221	NO 2002-6199	20021223

PRIORITY APPLN. INFO.:

US 2000-215323P	P	20000630
US 2000-252736P	P	20001122
US 2000-255956P	P	20001215
US 2001-268497P	P	20010213
US 2001-279779P	P	20010329
US 2001-295589P	P	20010604
WO 2001-US21012	W	20010629

OTHER SOURCE(S): MARPAT 136:102190

GI



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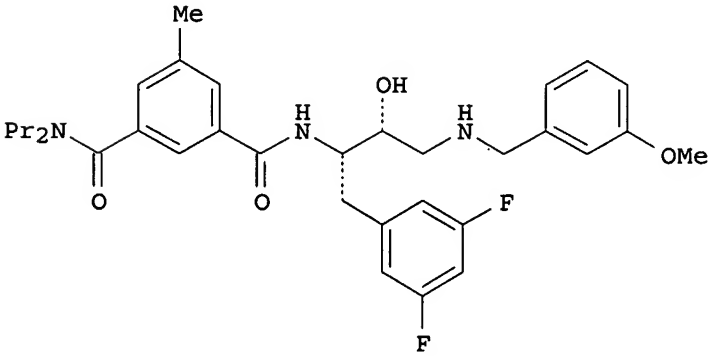


II

AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, (un)substituted alkyl, alkenyl, etc.; R3 = H, (un)substituted alkyl, alkenyl, etc.; R4 = XR; X = CO, SO2, a bond, etc.; R = Ph, naphthyl, indanyl, etc.; R5 = (un)substituted alkyl, (CH2)0-3cycloalkyl, etc.], useful in treating Alzheimer's disease and other similar diseases, were prepd. Thus, reacting (2R,3S)-3-amino-4-(3,5-difluorophenyl)-1-[(3-methoxybenzyl)amino]-2-butanol trifluoroacetate with 5-methyl-N,N-dipropylisophthalamic acid in the presence of Et3N, 1-hydroxybenzotriazole and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride in DMF

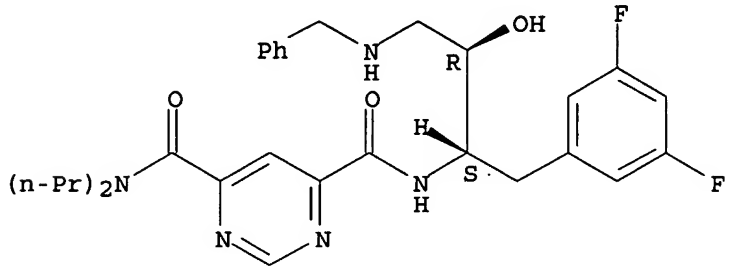
afforded (1S,2R)-II. The compds. I exhibit an IC50 of < 50 .mu.M against beta-secretase.

IT **388063-71-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted amines for treating Alzheimer's disease)

RN 388063-71-6 CAPLUS

CN 4,6-Pyrimidinedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-2-hydroxy-3-[(phenylmethyl)amino]propyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)

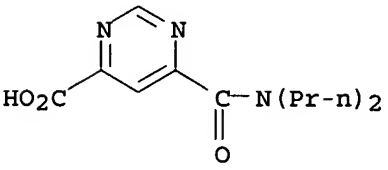
Absolute stereochemistry.



IT **388072-34-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of substituted amines for treating Alzheimer's disease)

RN 388072-34-2 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 6-[(dipropylamino)carbonyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:807797 CAPLUS

DOCUMENT NUMBER: 130:191413

TITLE: Identification of HIV-1 integrase inhibitors based on a four-point pharmacophore

AUTHOR(S): Hong, H.; Neamati, N.; Winslow, H. E.; Christensen, J. L.; Orr, A.; Pommier, Y.; Milne, G. W. A.

CORPORATE SOURCE: Laboratory Medicinal Chemistry, National Cancer Institut, National Institutes Health, MD, 20892, USA

SOURCE: Antiviral Chemistry & Chemotherapy (1998), 9(6), 461-472
CODEN: ACCHEH; ISSN: 0956-3202

PUBLISHER: International Medical Press

DOCUMENT TYPE: Journal

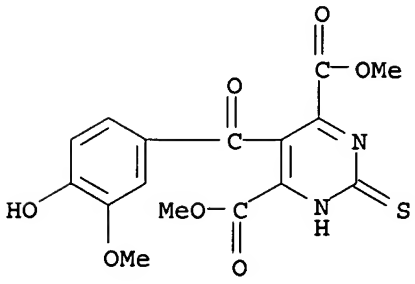
LANGUAGE: English

AB The rapid emergence of human immunodeficiency virus (HIV) strains resistant to available drugs implies that effective treatment modalities will require the use of a combination of drugs targeting different sites of the HIV life cycle. Because the virus cannot replicate without integration into a host chromosome, HIV-1 integrase (IN) is an attractive

therapeutic target. Thus, an effective IN inhibitor should provide addnl. benefit in combination chemotherapy. A four-point pharmacophore has been identified based on the structures of quinalizarin and purpurin, which were potent IN inhibitors using both a preintegration complex assay and a purified enzyme assay in vitro. Searching with this four-point pharmacophore in the 'open' part of the National Cancer Institute three-dimensional structure data-base produced 234 compds. contg. the pharmacophore. Sixty of these compds. were tested for their inhibitory activity against IN using the purified enzyme; 19 were active against IN with IC50 values of less than 100 .mu.M, among which 10 had IC50 values of less than 10 .mu.M. These inhibitors can further serve as leads, and studies are in progress to design novel inhibitors based on the results presented in this study.

IT **220751-87-1**, NSC 371068
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of HIV-1 integrase inhibitors based on a four-point pharmacophore in relation to antiviral activity)

RN 220751-87-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 1,2-dihydro-5-(4-hydroxy-3-methoxybenzoyl)-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:531603 CAPLUS
DOCUMENT NUMBER: 125:167964
TITLE: Preparation of bis(trifluoromethylpyrroloindolecarboxylic acid) and bis(trifluoromethylcyclopropapyrroloindolecarboxylic acid)derivatives as antitumor agents
INVENTOR(S): Fukuda, Yasumichi; Furuta, Kosuke; Oomori, Yasuo; Ko, Hiroyuki; Terajima, Atsuro
PATENT ASSIGNEE(S): Kyorin Seiyaku Kk, Japan; Sagami Chem Res
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08151380	A2	19960611	JP 1994-295276	19941129

PRIORITY APPLN. INFO.: JP 1994-295276 19941129
OTHER SOURCE(S): MARPAT 125:167964
GI

10/ 075,909

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I and II; R = linear or branched C1-6 alkyl; R1 = Q - Q4; wherein Z = NHCO-R3-CONH, NH, O, (CH2)n (n = 0-4), (CH:CH)m, (C.tplbond.C)m (m = 1,2), X3-(CH2)n-X3; or Z = NHCONH and X3 = O; wherein R3 = Q5, Q6; X1, X2, X4, X5 = H, OH, linear or branched C1-6 alkyl, alkyloxy, or alkyloxycarbonyl, (un)substituted aryloxy; X3 = NH, O; R2 = H, HO-protecting group, substituent hydrolyzable in vivo; Y = halo, arylsulfonyloxy, lower alkylsulfonyloxy, haloalkylsulfonyloxy, N3] and optically active isomers and pharmacol. acceptable salts thereof, which have low toxicity and potent and highly selective antitumor activity against solid tumors, even those with reduced sensitivity for anticancer agents, and also show antibacterial activity, are prepd. Thus, Me (S)-tert-butoxycarbonyl-1-chloromethyl-5-hydroxy-7-trifluoromethyl-1,2,3,6-tetrahydropyrrolo[3,2-e]indole-8-carboxylate was stirred with 3 M HCl/EtOAc at room temp. for 40 min and after distg. off the solvent, treated with 5,5'-(carbonyldiimino)bisbenzofuran-2-carboxylic acid and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, and stirred in DMF at room temp. overnight to give (S,S)-I [R = Me, R1 = Q (wherein Z = NHCONH, X1 = X2 = H, X3 = O), Y = Cl, R2 = H]. The latter compd. and (S,S)-I [R = Me, R1 = Q (wherein Z = single bond, X1 = X2 = H, X3 = NH), Y = Cl, R2 = H] in vitro showed IC50 of 0.31 and 0.0049 ng/mL against Hela S3 cells and in vivo inhibited the growth of colon 26 tumor transplanted in mice by 92% at 0.0156 mg/kg and 84% at 0.000977 mg/kg, resp.

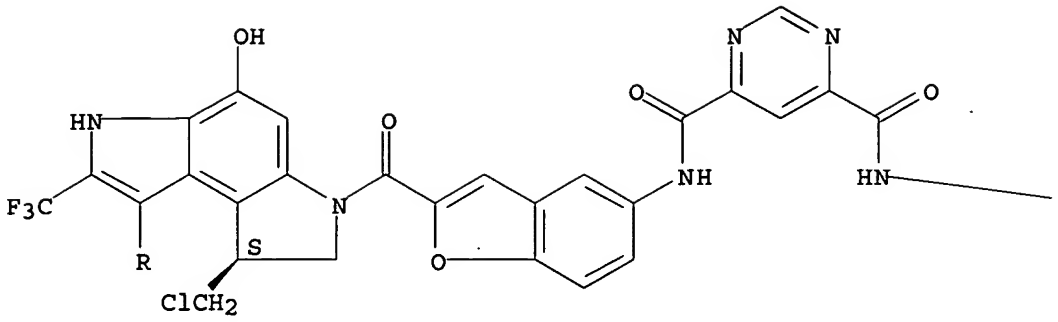
IT **180525-89-7P 180525-99-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of bis(trifluoromethylpyrroloindolecarboxylic acid) and bis(trifluoromethylcyclopropapyrroloindolecarboxylic acid)derivs. as antitumor agents)

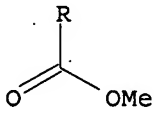
RN 180525-89-7 CAPLUS

CN Benzo[1,2-b:4,3-b']dipyrrole-1-carboxylic acid, 6,6'-[4,6-pyrimidinediylbis(carbonylimino-5,2-benzofurandiylcarbonyl)]bis[(8S)-8-(chloromethyl)-3,6,7,8-tetrahydro-4-hydroxy-2-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

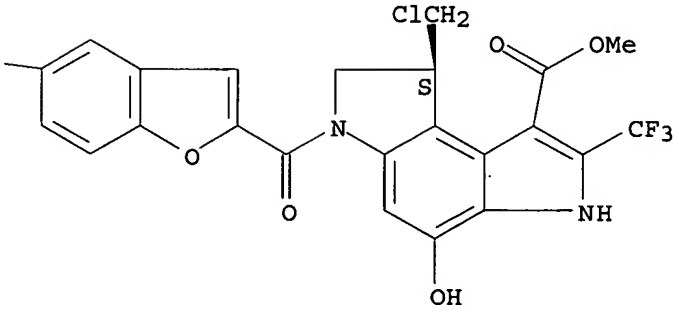
Absolute stereochemistry. Rotation (+).

PAGE 1-A





PAGE 1-B

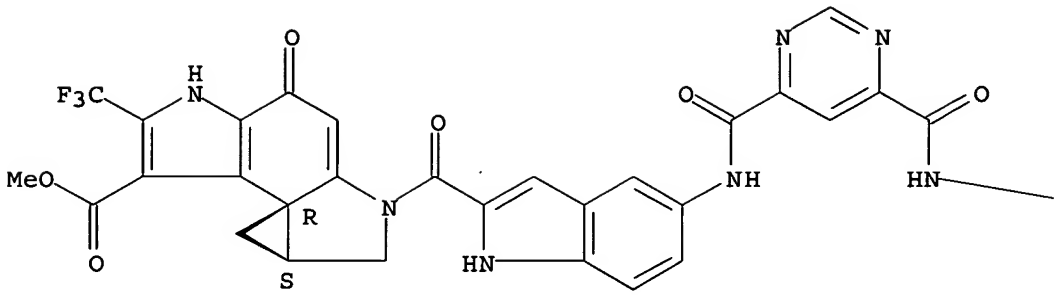


RN 180525-99-9 CAPLUS

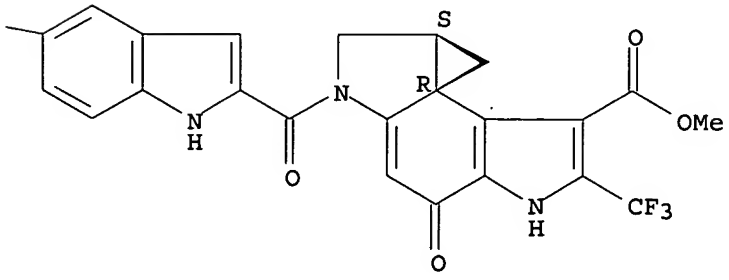
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[4,6-pyrimidinediylbis(carbonylimino-1H-indole-5,2-diylcarbonyl)]bis[1,2,4,5,8,8a-hexahydro-4-oxo-6-(trifluoromethyl)-, dimethyl ester, [7bR-[7bR*,8aR*(7'bR*,8'aS*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

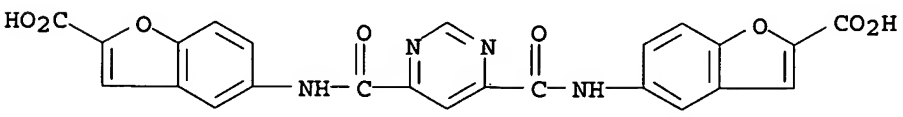
PAGE 1-A



PAGE 1-B



IT **180526-01-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of bis(trifluoromethylpyrroloindolecarboxylic acid) and bis(trifluoromethylcyclopropapyrroloindolecarboxylic acid)derivs. as antitumor agents)
RN 180526-01-6 CAPLUS
CN 2-Benzofurancarboxylic acid, 5,5'-[4,6-pyrimidinediylbis(carbonylimino)]bis- (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:640456 CAPLUS
DOCUMENT NUMBER: 123:285887
TITLE: Direct introduction of acyl and ethoxycarbonyl groups into pyrimidine ring through the trimethylstannyl derivatives
AUTHOR(S): Yamamoto, Yutaka; Ouchi, Hidekazu; Tanaka, Takuo; Morita, Yasuo
CORPORATE SOURCE: Tohoku Coll. Pharmacy, Sendai, 981, Japan

10/ 075,909

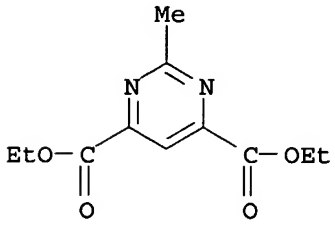
SOURCE: Heterocycles (1995), 41(6), 1275-90
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285887

AB The reactions of acylformyl chlorides with 2- and 4-trimethylstannylpyrimidine derivs. proceeded more smoothly than those of acyl chlorides giving the corresponding 2- and 4-acylpyrimidines. Employing Et chloroglyoxylate instead of the acylating agent yielded the (ethoxycarbonyl)pyrimidines. Similarly, the stepwise acylation and ethoxycarbonylation of bis(trimethylstannyl)pyrimidines provided pyrimidines having two different carbon functional groups.

IT **169259-22-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(acylation and ethoxycarbonylation of pyrimidines via trimethylstannyl intermediates)

RN 169259-22-7 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, 2-methyl-, diethyl ester (9CI) (CA INDEX NAME)



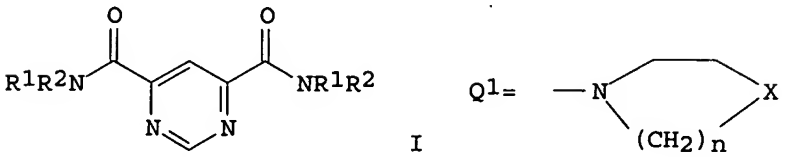
L3 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:471610 CAPLUS
DOCUMENT NUMBER: 115:71610
TITLE: Preparation of pyrimidine-4,6-dicarboxylic acid diamides as proline- and lysine hydroxylase inhibitors
INVENTOR(S): Baader, Ekkehard; Bickel, Martin; Guenzler-Pukall, Volkmar; Henke, Stephan
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 418797	A2	19910327	EP 1990-117894	19900918
EP 418797	A3	19910508		
EP 418797	B1	19940824		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DE 3931432	A1	19910404	DE 1989-3931432	19890921
ES 2062239	T3	19941216	ES 1990-117894	19900918
DD 295835	A5	19911114	DD 1990-344102	19900919
US 5130317	A	19920714	US 1990-584655	19900919
SU 1836359	A3	19930823	SU 1990-4831137	19900919
IL 95740	A1	19940731	IL 1990-95740	19900919
CA 2025799	AA	19910322	CA 1990-2025799	19900920
NO 9004114	A	19910322	NO 1990-4114	19900920
AU 9062698	A1	19910411	AU 1990-62698	19900920

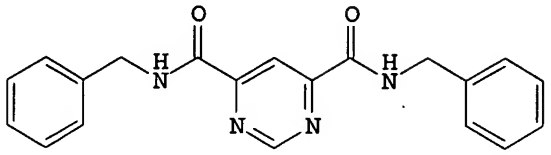
AU 633142	B2	19930121		
ZA 9007535	A	19910626	ZA 1990-7535	19900920
JP 03240776	A2	19911028	JP 1990-249018	19900920
PL 164989	B1	19941031	PL 1990-286972	19900920
HU 55002	A2	19910429	HU 1990-6007	19900921
HU 207853	B	19930628		

PRIORITY APPLN. INFO.: DE 1989-3931432 19890921
OTHER SOURCE(S): MARPAT 115:71610

GI



I



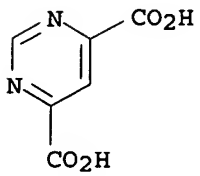
II

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, (benzo-annelated) cycloalkyl, (substituted) (hetero)aryl, amino; R2 = H, R1; R1R2N = Q1; R3 = H, (substituted) Ph, alkyl, alkenyl, alkynyl, alkoxycarbonyl, cycloalkyl; n = 1-3], were prepd. Thus, pyrimidine-4,6-dicarboxylic acid was refluxed .apprx.3 h with SOCl2 and cat. DMF in PhMe; the mixt. was cooled to 0-10.degree. and treated with PhCH2NH2 and Et3N followed by 12 h stirring at room temp. to give title compd. II. II at 50 mg/kg orally daily showed 21% redn. in CCl4-induced liver hydroxyproline concn. in rats.

IT **16490-02-1**, Pyrimidine-4,6-dicarboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, in prepn. of proline- and lysinehydroxylase inhibitors)

RN 16490-02-1 CAPLUS

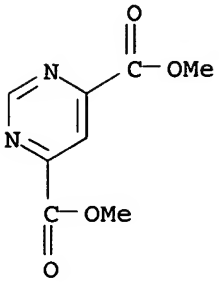
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **6345-43-3**, Dimethyl pyrimidine-4,6-dicarboxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrazinolysis of, in prepn. of proline- and lysinehydroxylase inhibitor)

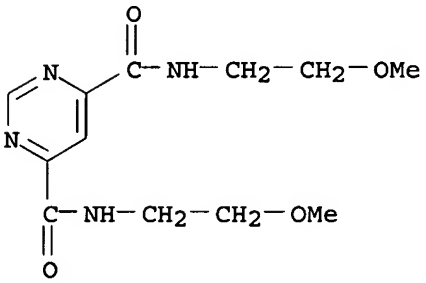
RN 6345-43-3 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

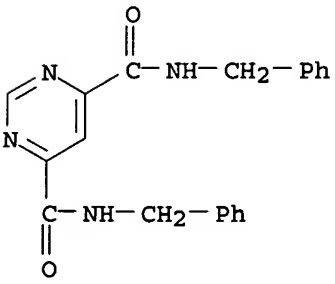


IT **135002-39-0P 135002-40-3P 135002-41-4P**
135002-43-6P 135002-44-7P 135002-46-9P
135002-47-0P 135002-48-1P 135002-49-2P
135002-50-5P 135002-51-6P 135002-52-7P
135002-53-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as proline- and lysinehydroxylase inhibitor)

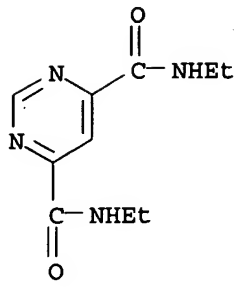
RN 135002-39-0 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(2-methoxyethyl)- (9CI) (CA INDEX NAME)



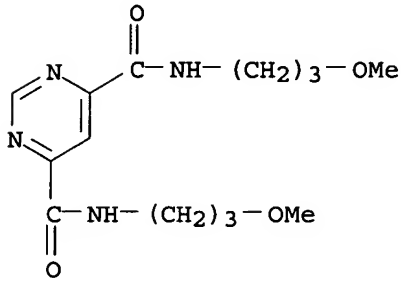
RN 135002-40-3 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



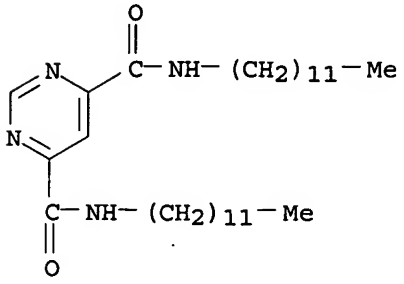
RN 135002-41-4 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-diethyl- (9CI) (CA INDEX NAME)



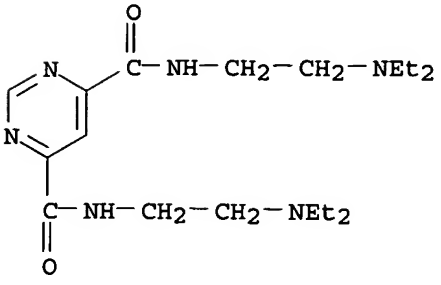
RN 135002-43-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(3-methoxypropyl)- (9CI) (CA INDEX NAME)



RN 135002-44-7 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-didodecyl- (9CI) (CA INDEX NAME)



RN 135002-46-9 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis[2-(diethylamino)ethyl]- (9CI) (CA INDEX NAME)



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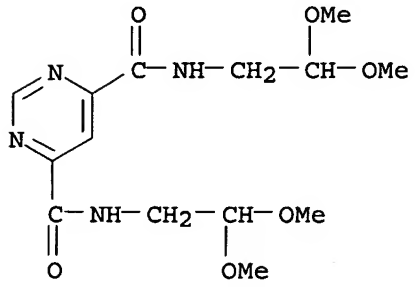
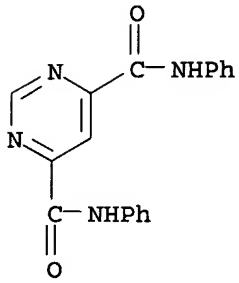
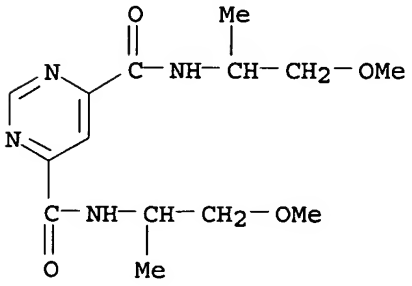
RN 135002-47-0 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(2,2-dimethoxyethyl)- (9CI) (CA INDEX NAME)



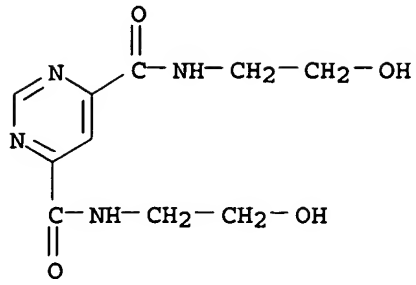
RN 135002-48-1 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-diphenyl- (9CI) (CA INDEX NAME)



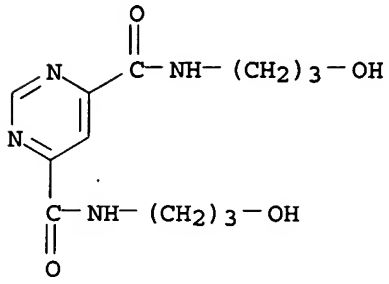
RN 135002-49-2 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(2-methoxy-1-methylethyl)- (9CI) (CA INDEX NAME)



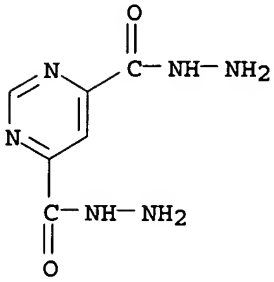
RN 135002-50-5 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



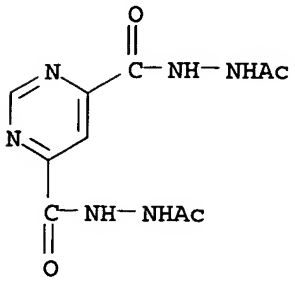
RN 135002-51-6 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, N,N'-bis(3-hydroxypropyl)- (9CI) (CA INDEX NAME)



RN 135002-52-7 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, dihydrazide (9CI) (CA INDEX NAME)



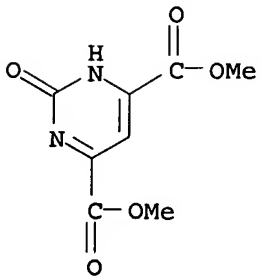
RN 135002-53-8 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, bis(2-acetylhydrazide) (9CI) (CA INDEX NAME)



L3 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:71644 CAPLUS
DOCUMENT NUMBER: 110:71644
TITLE: Mercaptan and dicarboxylate inhibitors of hamster dihydroorotase
AUTHOR(S): Christopherson, Richard I.; Schmalzl, Karl J.; Szabados, Eve; Goodridge, Richard J.; Harsanyi, Michael C.; Sant, Melissa E.; Algar, Elizabeth M.; Anderson, Janet E.; Armstrong, Alison; et al.
CORPORATE SOURCE: Dep. Biochem., Univ. Sydney, Sydney, 2006, Australia
SOURCE: Biochemistry (1989), 28(2), 463-70
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In mammals, dihydroorotase is part of a trifunctional protein, dihydroorotate synthetase, which catalyzes the 1st 3 reactions of de novo pyrimidine biosynthesis. Dihydroorotase catalyzes the formation of a peptidelike bond between the terminal ureido N and the .beta.-carboxyl group of N-carbamyl-L-aspartate to yield heterocyclic L-dihydroorotate. Combining structural features of the substrates with a thiol or carboxyl group in an appropriate position to coordinate the Zn bound at the catalytic site produces tight-binding inhibitors of Zn proteases, which have a catalytic mechanism similar to dihydroorotase. A similar compd., (4R)-2-oxo-6-thioxohexahydropyrimidine-4-carboxylate (L-6-thiodihydroorotate), was synthesized; this analog is a potent competitive inhibitor of dihydroorotase with a dissocn. const. (Ki) in the presence of excess Zn2+ of 0.17 .mu.M at pH 7.4. The potency of inhibition by L-6-thiodihydroorotate in the presence of divalent metal ions decreases in the order Zn2+ > Ca2+ > Co2+ > Mn2+ > Ni2+; L-6-thiodihydroorotate alone is less inhibitory and has a Ki of 0.85 .mu.M. 6-Thioorotate has a Ki of 82 .mu.M which decreases to 3.8 .mu.M in the presence of Zn2+. Zn2+ alone is a moderate inhibitor of dihydroorotase and does not enhance the potency of other inhibitors.

IT **114832-75-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 114832-75-6 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 1,2-dihydro-2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1988:571126 CAPLUS
DOCUMENT NUMBER: 109:171126
TITLE: Manufacture of liquid crystal polymers
INVENTOR(S): Hijikata, Kenji; Nakane, Toshio; Kageyama, Yukihiko
PATENT ASSIGNEE(S): Polyplastics Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

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CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63105027	A2	19880510	JP 1986-251425	19861022
JP 08030114	B4	19960327		

PRIORITY APPLN. INFO.: JP 1986-251425 19861022

AB Polymers which show anisotropic property on melting comprise .gtoreq.1 heterocyclic group in the main chain linkage in addn. to other structural components. Thus, 2,6-quinolinedicarboxylic acid 434, 2,6-naphthalenedicarboxylic acid 216, hydroquinone diacetate 582, and p-acetoxybenzoic acid 720 parts were heated to 260.degree. to remove AcOH, then at 260.degree. for 2.5 h and 280.degree. for 3 h with vigorous stirring, and finally heated in vacuo to provide a polymer (intrinsic viscosity 5.0) with flexural strength 1.410 (lengthwise) and 690 kg/cm2 (widthwise), and linear expansion coeff. -1.0 (lengthwise) and 3.1 cm/cm/.degree.C .times. 10-5.

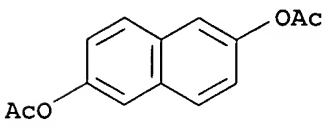
IT **117140-83-7P**
RL: PREP (Preparation)
(liq. crystals, prepn. of, with good mech. properties)

RN 117140-83-7 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, polymer with 4-(acetyloxy)benzoic acid, 1,4-benzenedicarboxylic acid and 2,6-naphthalenediyl diacetate (9CI) (CA INDEX NAME)

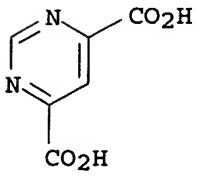
CM 1

CRN 22426-47-7
CMF C14 H12 O4



CM 2

CRN 16490-02-1
CMF C6 H4 N2 O4



CM 3

CRN 2345-34-8
CMF C9 H8 O4

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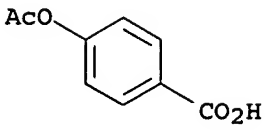
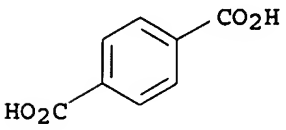


CM 4

CRN 100-21-0
CMF C8 H6 O4



L3 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1988:406545 CAPLUS
DOCUMENT NUMBER: 109:6545
TITLE: Preparation and testing of 2-oxo-4-carboxypyrimidines as neoplasm inhibitors and antimalarials
INVENTOR(S): Schmalzl, Karl John; Sharma, Suresh Chandra; Christopherson, Richard Ian
PATENT ASSIGNEE(S): University of Melbourne, Australia; University of Sydney
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 260057	A2	19880316	EP 1987-307744	19870902
EP 260057	A3	19890201		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 8777692	A1	19880331	AU 1987-77692	19860902
AU 595062	B2	19900322		
JP 63119471	A2	19880524	JP 1987-220095	19870901
US 4873228	A	19891010	US 1987-91761	19870901
ZA 8706552	A	19880525	ZA 1987-6552	19870902
PRIORITY APPLN. INFO.:			AU 1986-7811	19860902
			AU 1986-8161	19860922

OTHER SOURCE(S): MARPAT 109:6545
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R1, R2 = OH, peptide residue, alkoxy, alkoxymethyl, amino, any group able to be hydrolyzed in vivo to OH; R3, R4 = H, alkyl, hydroxyalkyl, tetrahydrofuranyl, tetrahydropyranyl, (acetylated) sugar residue, any group hydrolyzable in vitro to H; R5 = H, halo, alkyl; R6 = alkyl, 1-methyl-4-nitroimidazol-5-yl; A = H, B = COR2; AB = S] were prepd. as inhibitors of dihydroorotase. Di-Me 2-hydroxypyrimidine-4,6-dicarboxylate (prepn. given) was reduced with Zn/HOAc to give 28% di-Me 2-oxo-1,2,3,6-tetrahydropyrimidine-4,6-dicarboxylate, which was refluxed 30 min in 1M NaOH to give 50% 2-oxo-1,2,3,6-tetrahydropyrimidine-4,6-dicarboxylic acid (HDDP). HDDP bound dihydroorotase with a Ki of 0.48 .mu.m.

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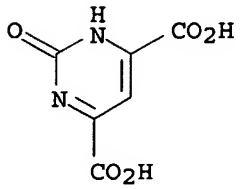
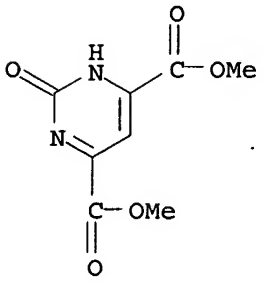
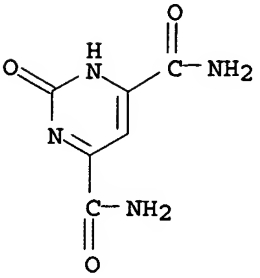
IT **114832-74-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of, in prepn. of drug)
RN 114832-74-5 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 1,2-dihydro-2-oxo- (9CI) (CA INDEX NAME)



IT **114832-75-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of, in prepn. of drug)
RN 114832-75-6 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 1,2-dihydro-2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



IT **114832-78-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as drug intermediate)
RN 114832-78-9 CAPLUS
CN 4,6-Pyrimidinedicarboxamide, 1,2-dihydro-2-oxo- (9CI) (CA INDEX NAME)



L3 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:26149 CAPLUS
DOCUMENT NUMBER: 94:26149
TITLE: Plant growth stimulant
INVENTOR(S): Karabanov, Yu. V.; Gridasova, V. I.; Cherkasov, V. M.;

10/ 075,909

	Prikazchikova, L. P.; Bragina, A. Sh.; Rybchenko, L. I.; Borisenko, V. P.
PATENT ASSIGNEE(S):	Institute of Organic Chemistry, Academy of Sciences, Ukrainian S.S.R., USSR
SOURCE:	U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1980, (6), 11. CODEN: URXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Russian
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 715080	T	19800215	SU 1978-2659696	19780821

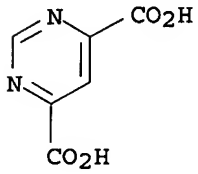
PRIORITY APPLN. INFO.: SU 1978-2659696 19780821

AB 4,6-Pyrimidinedicarboxylic acid (I) [**16490-02-1**] was used as a plant growth stimulant.

IT **16490-02-1**
RL: BIOL (Biological study)
(plant growth stimulant)

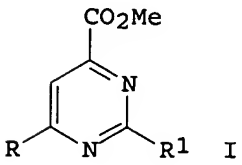
RN 16490-02-1 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:	1980:426380 CAPLUS
DOCUMENT NUMBER:	93:26380
TITLE:	Studies on pyrimidine derivatives. XVII. Synthesis of pyrimidine-4-carboxylic esters
AUTHOR(S):	Sakasai, Takeji; Sakamoto, Takao; Yamanaka, Hiroshi
CORPORATE SOURCE:	Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE:	Heterocycles (1979), 13(Spec. Issue), 235-8 CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	



AB Pyrimidinecarboxylates I (R = Me, R1 = H, Me, Ph) were obtained in 26-40% yield together with 7-11% I (R = CO2Me) by SeO2 oxidn. of 4,6-dimethylpyrimidines and esterification of the oxidn. mixt. I (R = H, Ph, R1 = Me) was similarly obtained in 58-65% yield.

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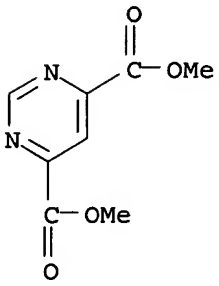
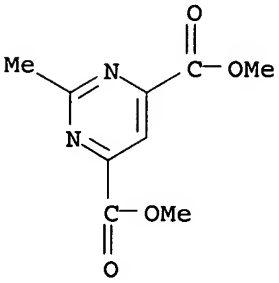
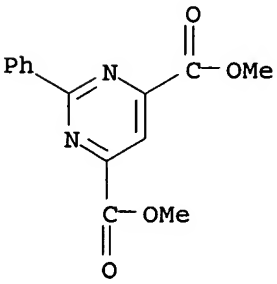
IT **6345-43-3P 73955-57-4P 73955-58-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 6345-43-3 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



RN 73955-57-4 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 2-methyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 73955-58-5 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, 2-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1977:602157 CAPLUS
DOCUMENT NUMBER: 87:202157
TITLE: Regular copolyamides. III. Preparation and characterization of regular aliphatic/aromatic copolyoxamides
AUTHOR(S): Stevenson, D.; Beeber, A.; Gaudiana, R.; Vogl, O.
CORPORATE SOURCE: Polym. Sci. Eng., Univ. Massachusetts, Amherst, MA,

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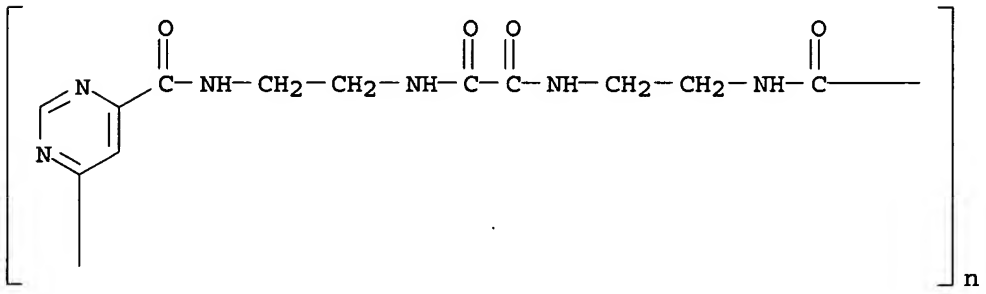
USA
SOURCE: Journal of Macromolecular Science, Chemistry (1977), A11(4), 779-809
CODEN: JMCHBD; ISSN: 0022-233X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Regular aliph.-arom. copolyoxamides were prepd. from diamineoxamides and arom. diacid chlorides by interfacial or by soln. polymn; soln. polymn. in CHCl3 or AcNMe2 is preferred for prepn. of large quantities of polymers but interfacial polymn. is most convenient for prepn. of polymers with high mol. wt. Arom. diacid chlorides used included: diacid chlorides of terephthalic acid, isophthalic acid, 2,6-pyridinedicarboxylic acid, 2 isomeric naphthalene dicarboxylic acids, 2 cyclohexanedicarboxylic acid isomers, as well as 1,1-cyclobutanedicarboxylic acid. Copolymers of diamineoxamides with mixts. of acid chlorides of isophthalic and pyridinedicarboxylic acid and isophthalic acid-tetrachloroterephthalic acid were also prepd. Most polymers are film-forming and are sol. in concd. H2SO4, CF3CO2H, and AcNMe2 (contg. several per cent LiCl). Several of these polymers gave dense or asym. membranes, particularly polymers from ethylenediamine as the aliph. diamine, particularly poly(iminoethyleneiminooxalyliminoethyleneiminoisophthaloyl) [58610-84-7]. Diamine oxamides with >2 amide groups in the mols. were prepd., and in 1 case polymers with arom. diacid chlorides were prepd. by interfacial polymn. All regular aliph.-arom. copolyoxamides were high melting and generally decomposed at >350.degree. without melting. They can, however, be fabricated from soln. into brittle fibers or into desalination membranes.

IT **63391-14-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 63391-14-0 CAPLUS
CN Poly[4,6-pyrimidinediylcarbonylimino-1,2-ethanediylimino(1,2-dioxo-1,2-ethanediyl)imino-1,2-ethanediyliminocarbonyl] (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1977:567966 CAPLUS
DOCUMENT NUMBER: 87:167966
TITLE: Pyrimidines. LXII. Some reactions of pyrimidine cyano derivatives
AUTHOR(S): Shkurko, O. P.; Mamaev, V. P.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1977), (6), 821-4
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

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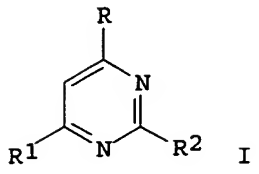


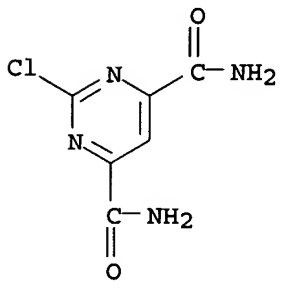
I

AB Pyrimidinecarbonitriles I (R = CN, R1 = Me, R2 = Cl; R = R1 = CN, R2 = Cl) were obtained in 24 and 28% yields by treatment of I (R = R1 = Me, R2 = OH, NH2) with NaNO2 and POCl3. Subsequent hydration with H2SO4 gave the corresponding amides. Treatment of I (R = R1 = CN, R2 = Cl) with NH3 gave 80 and 36% I (R = R1 = CN, R2 = NH2) and I (R = NH2, R1 = CN, R2 = Cl), resp.

IT **7150-30-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 7150-30-3 CAPLUS

CN 4,6-Pyrimidinedicarboxamide, 2-chloro- (9CI) (CA INDEX NAME)



L3 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1975:578072 CAPLUS

DOCUMENT NUMBER: 83:178072

TITLE: Effect of basicity of heterocyclic nitrogen on the conversion of heteroaromatic carboxylic acids to corresponding trichloromethyl compounds

AUTHOR(S): Takahashi, Kazuyuki; Kimura, Ikuo; Takei, Yutaka; Zaima, Tadataka; Mitsuhashi, Keiryo

CORPORATE SOURCE: Coll. Technol., Seikei Univ., Musashino, Japan

SOURCE: Nippon Kagaku Kaishi (1975), (9), 1530-4
CODEN: NKAKB8; ISSN: 0369-4577

DOCUMENT TYPE: Journal

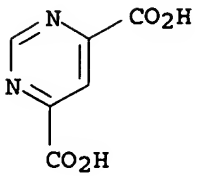
LANGUAGE: Japanese

AB The previously reported conversion of CO2H groups to CCl3 groups in imidazole- and pyridinecarboxylic acids (by reaction with PCl5 in excess SOCl2) was extended and correlated with basicity. Thus, the CO2H groups in 4-chloro- and 6-methylpicolinic acid were converted into CCl3 groups; 3- and 6-chloropicolinic acid and pyrazine-2,5-, pyrimidine-4,6-, and pyridazine-3,6-dicarboxylic acid gave only the corresponding carbonyl chlorides. Acids having pKa values higher than .apprx.3.5 were successfully converted to the trichloromethyl derivs.

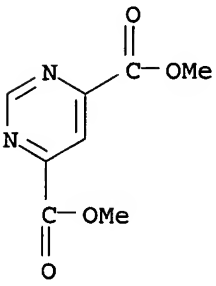
IT **16490-02-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of, basicity and)

RN 16490-02-1 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1974:569499 CAPLUS
DOCUMENT NUMBER: 81:169499
TITLE: Cycloaddition reactions with azabenzenes. VII. Reaction of pyrimidines with N,N-diethyl-1-propynylamine
AUTHOR(S): Neunhoffer, Hans; Werner, Gebhard
CORPORATE SOURCE: Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1974), (8), 1190-4
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The pyrimidinecarboxylates I (R-R3 = H or CO2Me) reacted with MeC.tplbond.CNEt2 via a Diels-Alder reaction with inverse electron demand to give .ltoreq.90% pyridine derivs. II (R4 .noteq. R5 = Me and NEt2). Rules for the orientation of the reactants are given.
IT **6345-43-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reaction of, with diethylpropynylamine)
RN 6345-43-3 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

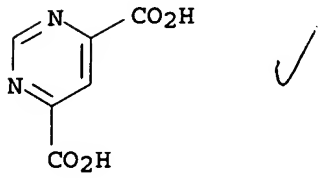


L3 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1974:500677 CAPLUS
DOCUMENT NUMBER: 81:100677
TITLE: Insecticidal activity of several pyrimidinecarboxylic acids and substituted 4,5,6-triaminopyrimidines
AUTHOR(S): Prikazchikova, L. P.; Kurilenko, L. K.; Rybchenko, L. I.; Cherkasov, V. M.; Dzyuban, A. D.; Protopopova, G. V.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Fiziologicheski Aktivnye Veshchestva (1966-1992) (1973), 5, 96-8
CODEN: FAVUAI; ISSN: 0533-1153
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Of 5 pyrimidinecarboxylic acids and esters and 4 derivs. of 4,5,6-pyrimidinetriamine, I [33968-03-5] had the greatest insecticidal

activity. Although all of the exptl. compds. were less active than chlorophos as contact insecticides and had lower systemic activities than that of Rogor I was sufficiently active upon contact with housefly imagoes, and systematically against spider mites, to merit consideration of its use against insects which have developed a resistance to organophosphorus insecticides.

IT **16490-02-1**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(insecticide)

RN 16490-02-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1973:466394 CAPLUS
DOCUMENT NUMBER: 79:66394
TITLE: 4,6-Pyrimidinedimethanol
INVENTOR(S): Matsumoto, Ikuo; Yoshizawa, Junji
PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 2 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

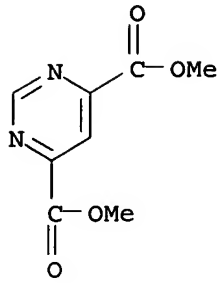
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48040783	A2	19730615	JP 1971-77840	19711006
JP 54027350	B4	19790910		

PRIORITY APPLN. INFO.: JP 1971-77840 19711006

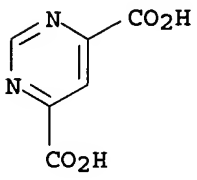
AB Alkyl 4,6-pyrimidinedicarboxylate was reduced with NaBH4 in EtOH in the presence of CaCl2. E.g., 5 g dimethyl 4,6-pyrimidinedicarboxylate was stirred 2 hr at 0-5.degree. in a mixt. of 1.5 g NaBH4, 2.2 g CaCl2, and EtOH to give 56% title compd.

IT **6345-43-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(redn. of)

RN 6345-43-3 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



L3 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1972:494976 CAPLUS
DOCUMENT NUMBER: 77:94976
TITLE: Infrared spectra of pyrimidinecarboxylic acids, and problems of their structure
AUTHOR(S): Titov, E. V.; Prikazchikova, L. P.; Rybchenko, L. I.; Cherkasov, V. M.; Rybachenko, V. I.
CORPORATE SOURCE: Donetsk. Inst. Fiz.-Org. Khim., Donetsk, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (6), 833-5
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The ir spectra of solid samples of 17 pyrimidinecarboxylic acids and of their solns. in dioxane and in CHCl3 were recorded. The frequencies of valence vibrations of CO2H groups, which did not participate in tautomerism were linearly correlated with acidity consts.: vCO = (1871 .+-. 7.5) - (40.6 .+-. 2.26) pKa.
IT **16490-02-1**
RL: PRP (Properties)
(ir spectrum of solid, structure in relation to)
RN 16490-02-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



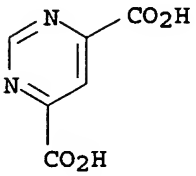
L3 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1967:469036 CAPLUS
DOCUMENT NUMBER: 67:69036
TITLE: Infrared spectra of some derivatives of pyrimidine-carboxylic acid
AUTHOR(S): Hermann, Theodore S.; Black, J. M.
CORPORATE SOURCE: Midwest Res. Inst., Kansas City, MO, USA
SOURCE: Applied Spectroscopy (1966), 20(6), 413-14
CODEN: APSPA4; ISSN: 0003-7028
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. Short and Thompson, CA 46: 9986e; Lord, et al., CA 51: 14423d. The KBr disk ir spectra of 36 pyrimidine-4-carboxylic acids substituted in the 2- and 6-positions with hydroxy, mercapto, or amino (Daves, et al., CA 55: 27343b) have been studied. The pyrimidine ring vibrations are tabulated

and the ranges of frequencies assigned to the ring modes are 1655-1565, 1470-1390, 1000-940, and 725-680 cm.-1

IT **16490-02-1**
RL: PRP (Properties)
(spectrum (ir) of)

RN 16490-02-1 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1964:404222 CAPLUS
DOCUMENT NUMBER: 61:4222
ORIGINAL REFERENCE NO.: 61:657g-h,658a-h,659a-b
TITLE: New pyrimidine syntheses
AUTHOR(S): Kroehnke, Fritz; Schmidt, Erhard; Zecher, Wilfried
CORPORATE SOURCE: Univ. Giessen, Germany
SOURCE: Ber. (1964), 97(4), 1163-75
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Three new routes are described for the synthesis of substituted pyrimidines in which C-2 was introduced through aromatic or heterocyclic aldehydes and the 2 N atoms of the pyrimidine nucleus through 2 mol. NH3 or NH4OAc (I)-AcOH. The 3 routes used arylidene 1,3-diketones, 2-halo 1,3-diketones, and phenacylcyclimonium salts, resp., as the starting materials. PhCH:CAc2 (1.81 cc.) in 12 cc. AcOH and 9 g. I treated dropwise at 60.degree. with 2 cc. BzH and kept 24 hrs. at room temp. yielded 1.48 g. 4,6-dimethyl-2-phenyl-5-benzylpyrimidine (II), needles, m. 96-7.degree. (MeOH). Hydrobenzamide (1.5 g.) in 10 cc. AcOH and 7 g. I treated dropwise at 60-70.degree. with 1.81 cc. PhCH:CAc2 and cooled after 2 hrs. yielded 1.51 g. II, m. 95-6.degree.. Ac2CH2 (0.51 cc.), 1.5 g. m-O2NC6H4CHO (III), 6 cc. AcOH, and 4.5 g. I kept 3 days at room temp. yielded 0.28 g. 4,6-dimethyl-2-(m-nitrophenyl)-5-(m-nitrobenzyl)pyrimidine (IV), needles, m. 200-1.degree. (repptd. from C5H5N with MeOH), which was also obtained in 55% yield from m-O2NC6H4CH:CAc2 and III. PhCH:CAc2 and III heated 1 hr. at 70.degree. and kept 24 hrs. at room temp. yielded 1.75 g. 2-(m-O2NC6H4) analog of II, needles, m. 131.degree. (repptd. from C5H5N with MeOH). A similar mixt. but with a larger excess of III heated 0.5 hr. at 60-70.degree. and kept 24 hrs. at room temp. yielded 0.5 g. IV, needles, m. 200-1.degree. and 0.6 g. 5-(m-O2NC6H4CH2) analog of II, needles, m. 125.degree. (EtOH). p-O2NC6H4CHO (V) (2.28 g.) in 12 cc. AcOH treated at 60-70.degree. with 1.81 cc. PhCH:CAc2 and 9 g. I and cooled after 0.5 hr. yielded after 24 hrs. 3.0 g. 2-(p-O2NC6H4) analog of II, yellow needles, m. 183.degree.. AcCH2COEt condensed with BzH yielded 70% PhCH:CAcCOEt (VI), b15, 188-91.degree.. VI (2.02 g.) and 1.6 g. 3-pyridine-carboxaldehyde in 12 cc. AcOH heated 40 min. with 9 g. I at 60-70.degree. and kept 24 hrs. yielded a product, which dissolved in 5 cc. MeOH, 1 cc. Me2CO, and 1 cc. Et2O and treated with picric acid in MeOH gave 2.7 g. picrate of 4-methyl-6-ethyl-5-benzyl-2-(3-pyridyl)pyrimidine (VII), yellow rodlets, m. 178-9.degree. (1:2 HCO-NMe2-EtOH); the picrate boiled briefly with a little dil. NH4OH gave VII, leaflets, m. 73-4.degree. (50% EtOH). 1,1-Diacetyl-2-(2-pyridyl)ethylene and p-ClC6H4CHO heated 0.5 hr. at 70-80.degree. and dild. after 15 min. with 4 cc. 50% MeOH gave 1.65 g. 4,6-dimethyl-5-(2-pyridylmethyl)-2-(p-

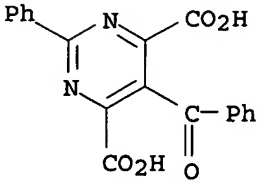
chlorophenyl)pyrimidine, prisms, m. 126-8.degree. (EtOH); picrate, yellow leaflets, m. 190-1.degree.. Quinoline-2-carboxaldehyde (VIII) condensed with Ac2CH2 yielded 1,1-diacetyl-2-(2-quinolyl)ethylene (IX), yellowish prisms, m. 145-6.degree. (EtOH). IX (1.18 g.) and 1.18 g. VIII in 6 cc. AcOH stirred 0.5 hr. with 4 g. I on the water bath gave 1.4 g. 4,6-dimethyl-5-(2-quinolylmethyl)-2-(2-quinolyl)pyrimidine, yellow needles, m. 270-1.degree. (C5H5N). II (1 g.), 4 cc. BzH, and 0.3 g. ZnCl2 heated 4 hrs. in a sealed vessel at 150.degree. gave 1.6 g. 2-phenyl-5-benzyl-4,6-distyrylpyrimidine, pale yellow needles, m. 197.5.degree. (C5H5N-MeOH); deep red and fluorescing in concd. H2SO4. II (2.25 g.) in 525 cc. 1% aq. KMnO4 refluxed 10 hrs. gave 1.5 g. 2-phenyl-5-benzoylpyrimidine-4,6-dicarhoxylic acid (X), needles, m. 184.degree. (decompn.) (50% aq. AcOH). X (0.8 g.), 6 cc. AcOH, and 1 cc. Ac2O refluxed 5 hrs. gave 0.55 g. 2-phenyl-5-benzoylpyrimidine, pink prisms, m. 91-2.degree. (C5H5N-MeOH); oxime, needles, m. 194-5.degree. (decompn.) (50% EtOH). ClCHAc2 (XI) (1.34 g.), 3.7 g. BzH, and 6 g. I in 8 cc. AcOH stirred 1 hr. at 70-80.degree. yielded 2.1 g. 2-phenyl-4,6-distyrylpyrimidine, needles and lancets, m. 160-1.degree. (PrOH), deep red in concd. H2SO4 and fluorescing in daylight. Analogous distyrylpyrimidines were obtained with p-MeOC6H4CHO (73%), 2,4-Cl2C6H3CHO (88%), and p-ClC6H4CHO (50%). XI (1.34 g.) and 2.27 g. V in 12 cc. AcOH refluxed 2 hrs. with 9 g. I gave 1.28 g. 4,6-dimethyl-2-(p-nitrophenyl)pyrimidine (XII), red, microcryst. powder, m. 157-60.degree. (C5H5N-MeOH). The crude XII treated with BzH and ZnCl2 at 150.degree. gave 80% 2-(p-nitrophenyl)-4,6-distyrylpyrimidine, light yellow needles and lancets, m. 258.degree. (C5H5N), red-violet in concd. H2SO4 fluorescing yellow-red in daylight. XI (1.34 g.), 2.27 g. V, 6 cc. AcOH, and 5 g. I heated 2 hrs. at 80-90.degree. yielded 1.5 g. 4-methyl-2-(p-nitrophenyl)-6-(p-nitrostyryl)pyrimidine and 2-(p-nitrophenyl)-4-styryl-6-(p-nitrostyryl)pyrimidine, light yellow lancets, m. 295.degree. (C5H5N), deep red in concd. H2SO4. AcBzCHCl (XIII) (0.98 g.), 1.5 g. V, 4 cc. AcOH, and 3 g. I heated 1.5 hrs. at 80-90.degree. gave 1.32 g. 6-Ph analog of XII, light yellow needles, 179-80.degree. (HCO-NMe2-MeOH). XIII with BzH gave similarly 50% 2,6-diphenyl-4-styrylpyrimidine, needles, m. 132.degree. (EtOH). III (4.6 g.), 2.23 g. AcCHClCOEt, 6 g. I, and 8 cc. AcOH refluxed 10 hrs. yielded 4.7 g. 6-ethyl-2-(m-nitrophenyl)-4-(m-nitrostyryl)pyrimidine, light yellow needles, m. 258-9.degree. (HCONMe2-EtOH), orange-yellow in concd. H2SO4. Bz2CHBr (1.5 g.), 1 cc. BzH, 4 cc. AcOH, and 3 g. I refluxed 3 hrs. yielded 0.6 g. 2,4,6-triphenylpyrimidine (XIV), needles, m. 185-6.degree. (EtOH). p-BrC6H4COCH2Bz brominated gave p-BrC6H4COCHBrBz (XV), needles, m. 120.degree. (CHCl3-ligroine). XV (1.9 g.), 1 cc. BzH, 3 g. I, and 4 cc. AcOH heated 3 hrs. on the water bath gave 1.2 g. 2,4-diphenyl-6-(p-bromophenyl)pyrimidine, rodlets, m. 166.degree. (EtOH). Bz2CHBr (3 g.), 2.2 g. III, 6 g. I, and 8 cc. AcOH heated 5 hrs. on the water bath yielded 2.3 g. 2-(m-O2NC6H4) analog of XIV, needles, m. 193.degree. (PrOH). Bz2CHOAc (1.41 g.), 1 cc. BzH, 3 g. NH4OAc, and 4 cc. AcOH refluxed 14 hrs. gave 0.15 g. XIV, needles, m. 185-6.degree. (EtOH). BzClCHCO2Et (2.26 g.), 2.25 g. III, 6 g. I, and 8 cc. AcOH refluxed 7 hrs. gave 0.5 g. 6-hydroxy-4-phenyl-2-(m-nitrophenyl)pyrimidine, pale yellow needles and rodlets, m. 271.degree. (HCONMe2-MeOH); the mother liquor gave 2 products, needles, m. 308-9.degree. and m. 324.degree.. ClCH(CONH2)2(XVI) (1.36 g.) and 1.2 cc. p-MeOC6H4CHO in 4 g. I and 5 cc. AcOH refluxed 4 hrs. gave 0.5 g. 4,6-diamino-2-(p-methoxy-phenyl)pyrimidine-2AcOH.1/3H2O, light pink needles, m. 234.degree., and 1.3 g. 4-amino-2-(p-methoxyphenyl)-5-carbamoyl-3-oxazoline-AcOH.1/3H2O (XVII), lancets, m. 216.degree. (PrOH). XVI with cumienaldehyde gave 15% 2-(p-cumyl) analog of XVII, rodlets, m. 237.degree. (MeOH). BrCH(CONMe)2 (2 g.), 1.5 cc. BzH, 4 g. I, and 5 cc. AcOH refluxed 7 hrs. yielded 0.7 g. 4-methyl-amino-2-phenyl-5-methylcarbamoyl-3-oxazoline-AcOH.0.5H2O, needles, m. 223-5.degree. (EtOH). N-Phenacylpyridinium bromide (2.78 g.), 3.78 g. V, 8 cc. AcOH, and 6 g. I refluxed 1.5 hrs. gave 3.1 g. 6-phenyl-2,4-bis(p-nitrophenyl)pyrimidine (XVIII), yellow lancets, m. 293-4.degree. (HCONMe2). N-Acetonylpyridinium

bromide (1.1 g.), 3 g. V, 7 cc. AcOH, and 4 g. I refluxed 20 min. yielded 1.25 g. 2,4-bis(p-nitrophenyl)-6-(p-nitrostyryl)pyrimidine, light yellow crystals, m. 348-54.degree. (HCONMe2), yellow-orange in concd. H2SO4. N-Phenacylisoquinolinium bromide with V gave 45% XVIII, m. 293-4.degree.. N-Phenacylquinolinium bromide with V gave 5% XVIII, prisms and rodlets, m. 293-4.degree.. [BzCH2SMe2]Br with V yielded 3.5 g. XVIII, prisms, m. 293-4.degree..

IT **94374-98-8**, 4,6-Pyrimidinedicarboxylic acid, 5-benzoyl-2-phenyl-
(prepn. of)

RN 94374-98-8 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, 5-benzoyl-2-phenyl- (7CI) (CA INDEX NAME)



L3 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1964:71442 CAPLUS

DOCUMENT NUMBER: 60:71442

ORIGINAL REFERENCE NO.: 60:12602a-b

TITLE: Stimulating plant growth

INVENTOR(S): Nickell, Louis G.

PATENT ASSIGNEE(S): Chas. Pfizer & Co., Inc.

SOURCE: 4 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3118754		19640121	US	19611010

AB Tests on duckweed, barley, and cucumbers showed a 200-300% increase in wet wt. after 7 days growth when treated with substituted pyrimidines, e.g., 4,6-pyrimidinedicarboxylic acid, its di-Me ester, 4-hydroxy-2-mercapto-6-propylpyrimidine, 4-hydroxy-2-mercapto-6-aminopyrimidine, 4-hydroxy-2-mercapto-6-aminopyrimidine, or 4-hydroxy-2-mercapto-5,6-dimethylpyrimidine. The addn. of gibberellic acid increases growth still more.

IT **6345-43-3**, 4,6-Pyrimidinedicarboxylic acid, dimethyl ester
16490-02-1, 4,6-Pyrimidinedicarboxylic acid
(as plant regulator)

RN 6345-43-3 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid, dimethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

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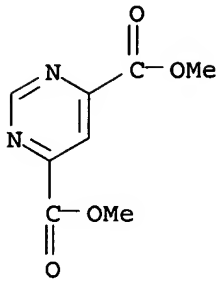
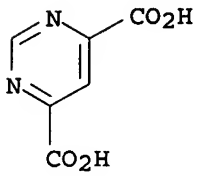


RN 16490-02-1 CAPLUS
CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1959:77812 CAPLUS
DOCUMENT NUMBER: 53:77812
ORIGINAL REFERENCE NO.: 53:14110d-i,14111a-c
TITLE: Pyrimidines. X. Pyrimidine, 4,6-dimethylpyrimidine, and their 1-oxides
AUTHOR(S): Hunt, R. R.; McOmie, J.F. W.; Sayer, E. R.
CORPORATE SOURCE: Univ. Bristol, UK
SOURCE: Journal of the Chemical Society, Abstracts (1959) 525-30
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

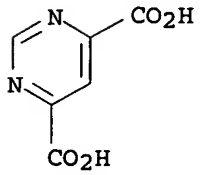
AB cf. C.A. 51, 12925d. A convenient 4-stage synthesis of pyrimidine has been devised starting with CH2Ac2 and thiourea. Concd. HCl (250 ml.) added to a 76 g. thiourea suspended in 120 g. CH2Ac2 and 2500 ml. EtOH, and the mixt. refluxed 2 hrs., then cooled, yielded 80% 2-mercapto-4,6-dimethylpyrimidine-HCl (I). Reworking the mother liquor increased the yield to 90%. I (90 g.) in 600 ml. EtOH desulfurized by refluxing 4 hrs. with 180 g. Raney Ni and 30 ml. concd. HCl, the filtrate mixed with Et2O, powd. NaOH added until the mixt. was alk., the liquid decanted, the solid ground with more Et2O until about 500 ml. ext. was obtained and the ext. fractionated gave 25-30 g. 4,6-dimethylpyrimidine (II), b758 154.degree., m. 24-6.degree.; methiodide m. 220-2.degree. (decompn., EtOH). The yield of II was not increased significantly by first converting I to 4,6-dimethyl-2-(methylthio)pyrimidine before desulfurization. KMnO4 (90 g.) in 550 ml. hot H2O added during 3 hrs. to a stirred soln. of 15 g. II in 50 ml. H2O contg. 3.6 g. NaOH at 70-80.degree., the MnO2 filtered off, the filtrate concd. to 100 ml., and concd. HCl added until the pH was 2-3 gave on cooling an av. yield of 60% 4,6-pyrimidinedicarboxylic acid (III) dihydrate, m. 210-11.degree. (decompn.). The dihydrate (46 g.) dried 1 week at 60.degree. gave 38 g. III, m. 218.degree. (decompn.). III (38 g.) added portionwise to 50 g. dry redistd. Ph2O in an oil bath at 240.degree. was rapidly decarboxylated to 60% pyrimidine (IV), b. 124-8.degree.. Bromination of II in glacial HOAc gave 39% 4,6-bis(tribromomethyl)pyrimidine, m. 125-6.degree. (ligroine, b. 60-80.degree.), .lambda. (EtOH) 267 m.mu., log .epsilon.

3.89, which, boiled with AgNO3 in HOAc, yielded 24% III, but the over-all yield via this route was lower than the method above. III di-Me ester m. 82-3.degree. (ligroine, b. 60-80.degree., sublimes), .lambda. (EtOH) 269, 320 m.mu., log .epsilon. 3.80, 2.46. A 2-stage synthesis of IV was attempted by first condensing CH2[CH(OEt)2]2 with thiourea in hot EtOH and concd. HCl to 66% 2-mercaptopyrimidine (V), m. 229-30.degree. (decompn., EtOH-H2O). The desulfurization of V was unsatisfactory as was that of 2-(pyrimidylthio)acetic acid, m. 199-200.degree. (H2O), prepd. in 60% yield from V and ClCH2CO2H. CH2[CH(OEt)2]2 added to a warm soln. of urea in EtOH and HCl and stirred 1 hr. at 30-40.degree., then cooled to 0.degree., gave 2-hydroxypyrimidine-HCl, m. 210.degree., converted by Na2CO3 to the base, m. 179-81.degree. (EtOAc). Attempts to condense the latter with benzamidine were unsuccessful. Concd. HCl (62 ml.) and 29 g. CH.tplbond.CCH:CHCH:CHOMe added to 25.5 g. thiourea in 275 ml. EtOH and the mixt. boiled 6 hrs. yielded 43.8 g. 2-mercapto-4-methylpyrimidine-HCl (V). V (1.6 g.) and 1.2 g. NaOH in 10 ml. H2O added to 1 g. ClCH2CO2H in 3 ml. H2O neutralized with Na2CO3, and the mixt. acidified after 4 days with dil. HCl gave 0.75 g. 4-methyl-2-(pyrimidylthio)acetic acid, m. 191.degree. (H2O). Water-wet Raney Ni (20 g.) added to 8 g. V in 75 ml. H2O which had been neutralized by Na2CO3, then refluxed 3 hrs., and the Et2O ext. of the filtrate distd. gave 0.9 g. 4-methylpyrimidine, b763 139-40.degree.; HgCl2 adduct m. 198-220.degree.; picrate m. 130-1.degree.. I (10.8 g.) in 60 ml. HOAc treated 3 hrs. with 10 ml. H2O2 at 70-80.degree. and worked up gave 7.1 g. 4,6-dimethylpyrimidine 1-oxide (VI), m. 113-15.degree.; picrate, m. 86.degree. (EtOH); HgCl2 adduct m. 158.degree. (H2O). VI (3.3 g.) and 5.0 g. p-MeC6H4SO2Cl in 20 ml. C6H6 kept at room temp. 0.5 hrs., the C6H6 removed, the residual oil heated on a H2O bath 1 hr., washed with Et2O, aq. NaHCO3 added, the mixt. extd. with CHCl3, and the ext. distd. in vacuo gave an unstable oil forming with picric acid 4-chloromethyl-6-methylpyrimidine picrate, m. 115.degree.. Ac2O added to 2.5 g. VI yielded 0.9 g. 4-acetoxymethyl-6-methylpyrimidine, b15 100-10.degree. (bath temp.); picrate m. 135-6.degree. (EtOH). IV also treated with H2O2 gave 9% pyrimidine 1-oxide, m. 89-91.degree.; picrate m. 84-5.degree.; HgCl2 adduct m. 161-2.degree.. 2-Chloro-4,6-dimethylpyrimidine (15 g.) added to 2.5 g. Na in 75 ml. PhCH2OH and boiled 4 hrs. yielded 14.7 g. 2-benzyloxy-4,6-dimethylpyrimidine, b2.5 160-5.degree..

IT **16490-02-1**, 4,6-Pyrimidinedicarboxylic acid
(and derivs.)

RN 16490-02-1 CAPLUS

CN 4,6-Pyrimidinedicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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L1 STRUCTURE UPLOADED

L2 118 S L1 FUL

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10/ 075,909

FILE 'CAPLUS' ENTERED AT 11:15:52 ON 28 OCT 2003
L3 27 S L2

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	123.72	274.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-17.58	-17.58

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